



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:23 PM GMT

PDB ID : 1JTS
Title : DNA PROTECTION AND BINDING BY E. COLI DPS PROTEIN
Authors : Luo, J.; Liu, D.; White, M.A.; Fox, R.O.
Deposited on : 2001-08-22
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

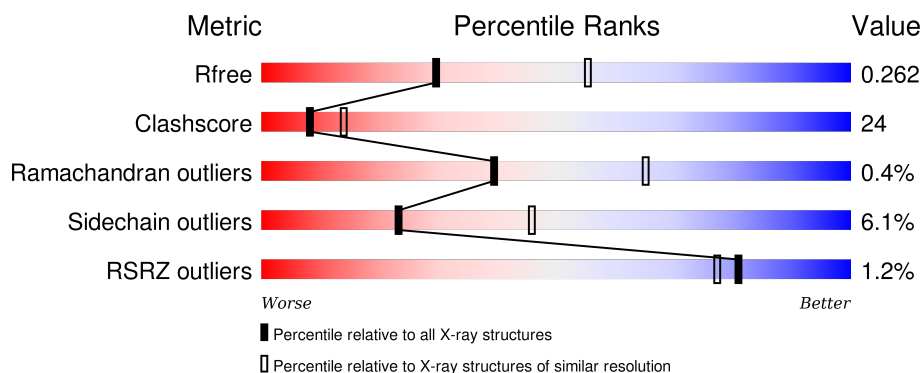
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	167	<div> <div>50%</div> <div>40%</div> <div>7%</div> </div>
1	B	167	<div> <div>48%</div> <div>41%</div> <div>7%</div> </div>
1	C	167	<div> <div>2%</div> <div>50%</div> <div>40%</div> <div>8%</div> </div>
1	D	167	<div> <div>4%</div> <div>51%</div> <div>38%</div> <div>8%</div> </div>
1	E	167	<div> <div>59%</div> <div>32%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	167	
1	G	167	
1	H	167	
1	I	167	
1	J	167	
1	K	167	
1	L	167	
1	M	167	
1	N	167	
1	O	167	
1	P	167	
1	Q	167	
1	R	167	
1	S	167	
1	T	167	
1	U	167	
1	V	167	
1	W	167	
1	X	167	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRS	G	303	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29850 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 DNA PROTECTION DURING STARVATION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1224	770	215	235	4			
1	B	155	Total	C	N	O	S	0	0	0
			1224	770	215	235	4			
1	C	154	Total	C	N	O	S	0	0	0
			1216	766	213	233	4			
1	D	154	Total	C	N	O	S	0	0	0
			1216	766	213	233	4			
1	E	156	Total	C	N	O	S	0	0	0
			1231	774	216	237	4			
1	F	155	Total	C	N	O	S	0	0	0
			1224	770	215	235	4			
1	G	155	Total	C	N	O	S	0	0	0
			1224	770	215	235	4			
1	H	154	Total	C	N	O	S	0	0	0
			1216	766	213	233	4			
1	I	154	Total	C	N	O	S	0	0	0
			1216	766	213	233	4			
1	J	158	Total	C	N	O	S	0	0	0
			1245	783	219	239	4			
1	K	154	Total	C	N	O	S	0	0	0
			1216	766	213	233	4			
1	L	155	Total	C	N	O	S	0	0	0
			1224	770	215	235	4			
1	M	156	Total	C	N	O	S	0	0	0
			1231	774	216	237	4			
1	N	156	Total	C	N	O	S	0	0	0
			1231	774	216	237	4			
1	O	156	Total	C	N	O	S	0	0	0
			1231	774	216	237	4			
1	P	154	Total	C	N	O	S	0	0	0
			1216	766	213	233	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	154	Total	C	N	O	S	0	0	0
			1216	766	213	233	4			
1	R	156	Total	C	N	O	S	0	0	0
			1231	774	216	237	4			
1	S	156	Total	C	N	O	S	0	0	0
			1231	774	216	237	4			
1	T	156	Total	C	N	O	S	0	0	0
			1231	774	216	237	4			
1	U	157	Total	C	N	O	S	0	0	0
			1236	777	217	238	4			
1	V	155	Total	C	N	O	S	0	0	0
			1224	770	215	235	4			
1	W	156	Total	C	N	O	S	0	0	0
			1231	774	216	237	4			
1	X	156	Total	C	N	O	S	0	0	0
			1231	774	216	237	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	CYS	ASP	ENGINEERED	UNP P0ABT2
A	78	ALA	ASP	ENGINEERED	UNP P0ABT2
B	75	CYS	ASP	ENGINEERED	UNP P0ABT2
B	78	ALA	ASP	ENGINEERED	UNP P0ABT2
C	75	CYS	ASP	ENGINEERED	UNP P0ABT2
C	78	ALA	ASP	ENGINEERED	UNP P0ABT2
D	75	CYS	ASP	ENGINEERED	UNP P0ABT2
D	78	ALA	ASP	ENGINEERED	UNP P0ABT2
E	75	CYS	ASP	ENGINEERED	UNP P0ABT2
E	78	ALA	ASP	ENGINEERED	UNP P0ABT2
F	75	CYS	ASP	ENGINEERED	UNP P0ABT2
F	78	ALA	ASP	ENGINEERED	UNP P0ABT2
G	75	CYS	ASP	ENGINEERED	UNP P0ABT2
G	78	ALA	ASP	ENGINEERED	UNP P0ABT2
H	75	CYS	ASP	ENGINEERED	UNP P0ABT2
H	78	ALA	ASP	ENGINEERED	UNP P0ABT2
I	75	CYS	ASP	ENGINEERED	UNP P0ABT2
I	78	ALA	ASP	ENGINEERED	UNP P0ABT2
J	75	CYS	ASP	ENGINEERED	UNP P0ABT2
J	78	ALA	ASP	ENGINEERED	UNP P0ABT2
K	75	CYS	ASP	ENGINEERED	UNP P0ABT2
K	78	ALA	ASP	ENGINEERED	UNP P0ABT2
L	75	CYS	ASP	ENGINEERED	UNP P0ABT2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	78	ALA	ASP	ENGINEERED	UNP P0ABT2
M	75	CYS	ASP	ENGINEERED	UNP P0ABT2
M	78	ALA	ASP	ENGINEERED	UNP P0ABT2
N	75	CYS	ASP	ENGINEERED	UNP P0ABT2
N	78	ALA	ASP	ENGINEERED	UNP P0ABT2
O	75	CYS	ASP	ENGINEERED	UNP P0ABT2
O	78	ALA	ASP	ENGINEERED	UNP P0ABT2
P	75	CYS	ASP	ENGINEERED	UNP P0ABT2
P	78	ALA	ASP	ENGINEERED	UNP P0ABT2
Q	75	CYS	ASP	ENGINEERED	UNP P0ABT2
Q	78	ALA	ASP	ENGINEERED	UNP P0ABT2
R	75	CYS	ASP	ENGINEERED	UNP P0ABT2
R	78	ALA	ASP	ENGINEERED	UNP P0ABT2
S	75	CYS	ASP	ENGINEERED	UNP P0ABT2
S	78	ALA	ASP	ENGINEERED	UNP P0ABT2
T	75	CYS	ASP	ENGINEERED	UNP P0ABT2
T	78	ALA	ASP	ENGINEERED	UNP P0ABT2
U	75	CYS	ASP	ENGINEERED	UNP P0ABT2
U	78	ALA	ASP	ENGINEERED	UNP P0ABT2
V	75	CYS	ASP	ENGINEERED	UNP P0ABT2
V	78	ALA	ASP	ENGINEERED	UNP P0ABT2
W	75	CYS	ASP	ENGINEERED	UNP P0ABT2
W	78	ALA	ASP	ENGINEERED	UNP P0ABT2
X	75	CYS	ASP	ENGINEERED	UNP P0ABT2
X	78	ALA	ASP	ENGINEERED	UNP P0ABT2

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	G	1	Total	C	N	O	0	0
			8	4	1	3		
2	G	1	Total	C	N	O	0	0
			8	4	1	3		
2	H	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	H	1	Total	C	N	O	0	0
			8	4	1	3		
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	L	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	M	1	Total	C	N	O	0	0
			8	4	1	3		
2	W	1	Total	C	N	O	0	0
			8	4	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	W	1	Total 8	C 4	N 1	O 3	0	0
2	T	1	Total 8	C 4	N 1	O 3	0	0
2	P	1	Total 8	C 4	N 1	O 3	0	0
2	P	1	Total 8	C 4	N 1	O 3	0	0
2	R	1	Total 8	C 4	N 1	O 3	0	0
2	T	1	Total 8	C 4	N 1	O 3	0	0
2	M	1	Total 8	C 4	N 1	O 3	0	0
2	P	1	Total 8	C 4	N 1	O 3	0	0
2	X	1	Total 8	C 4	N 1	O 3	0	0
2	Q	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
3	B	8	Total 8	O 8	0	0
3	C	8	Total 8	O 8	0	0
3	D	8	Total 8	O 8	0	0
3	E	10	Total 10	O 10	0	0
3	F	12	Total 12	O 12	0	0
3	G	4	Total 4	O 4	0	0
3	H	4	Total 4	O 4	0	0
3	I	8	Total 8	O 8	0	0

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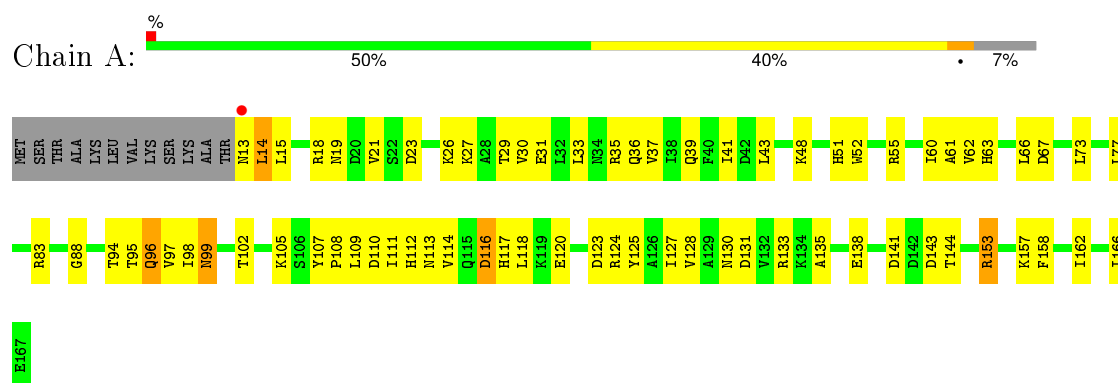
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	6	Total 6	O 6	0	0
3	K	5	Total 5	O 5	0	0
3	L	8	Total 8	O 8	0	0
3	M	11	Total 11	O 11	0	0
3	N	12	Total 12	O 12	0	0
3	O	11	Total 11	O 11	0	0
3	P	3	Total 3	O 3	0	0
3	Q	7	Total 7	O 7	0	0
3	R	10	Total 10	O 10	0	0
3	S	11	Total 11	O 11	0	0
3	T	16	Total 16	O 16	0	0
3	U	10	Total 10	O 10	0	0
3	V	11	Total 11	O 11	0	0
3	W	27	Total 27	O 27	0	0
3	X	22	Total 22	O 22	0	0

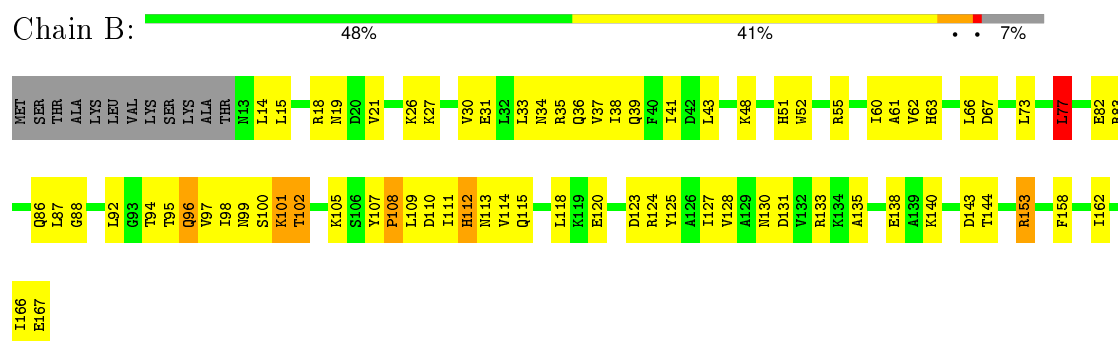
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

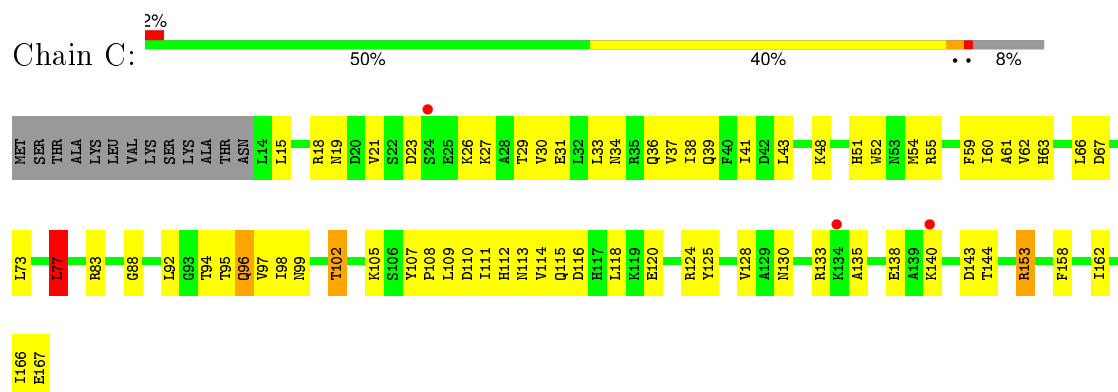
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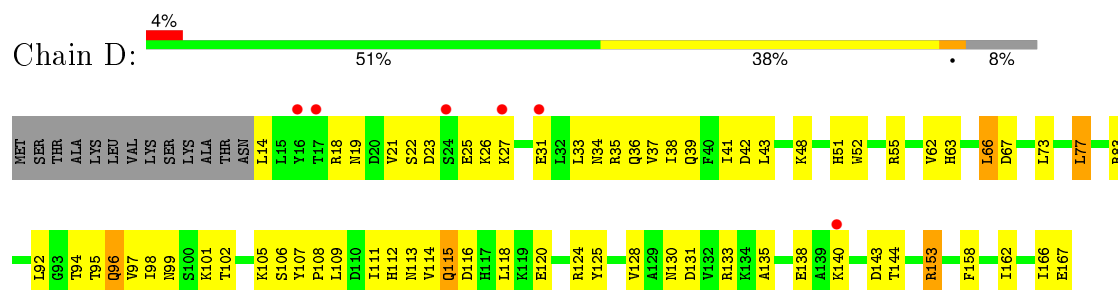
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



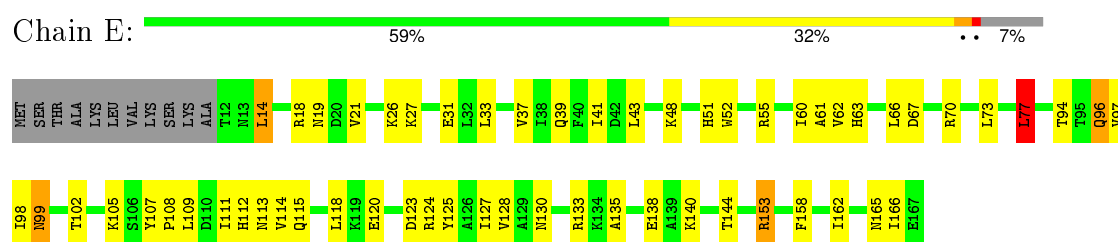
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



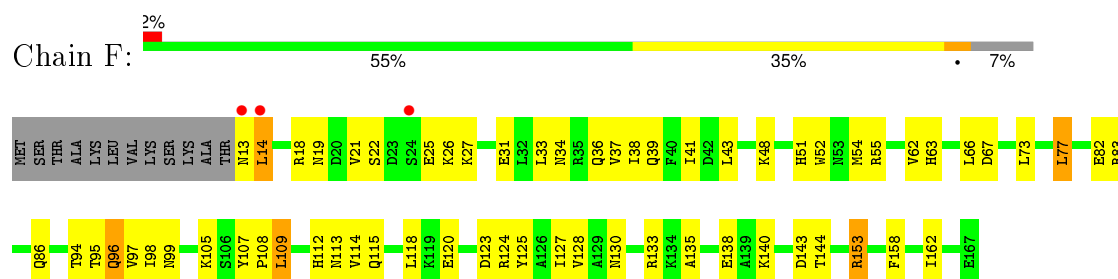
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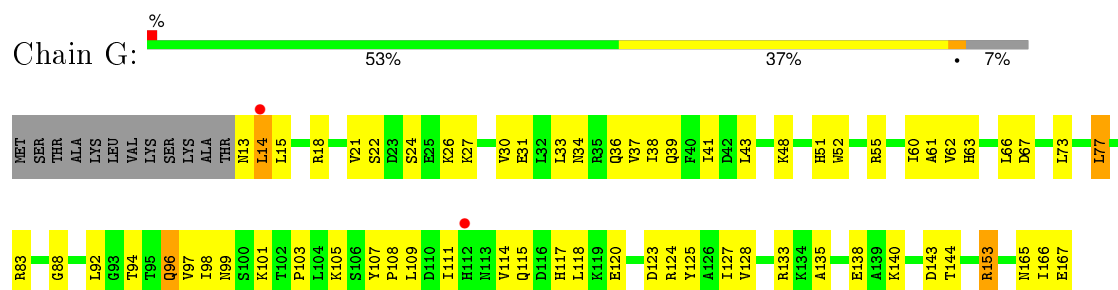
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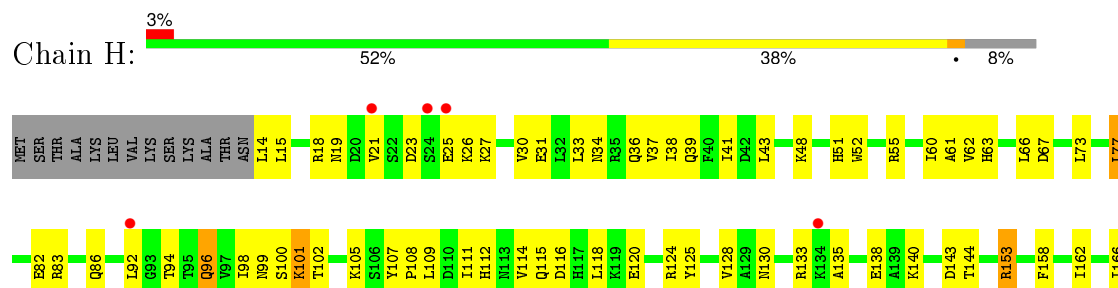
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

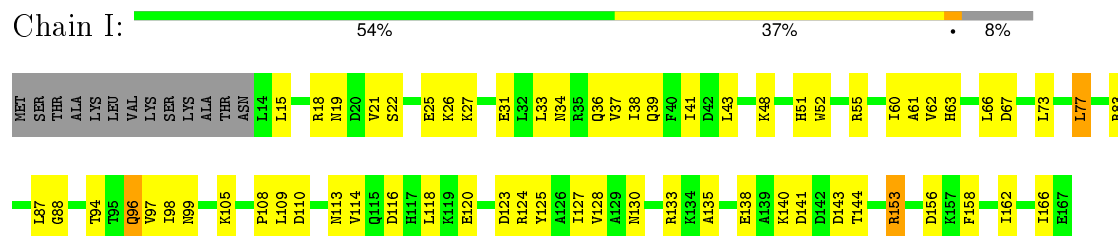


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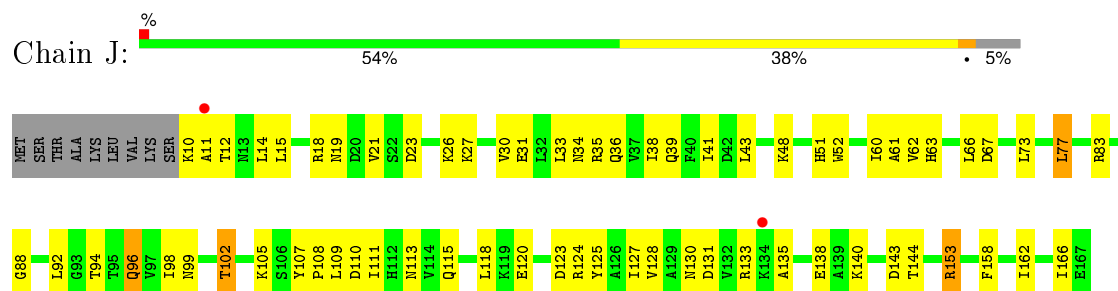


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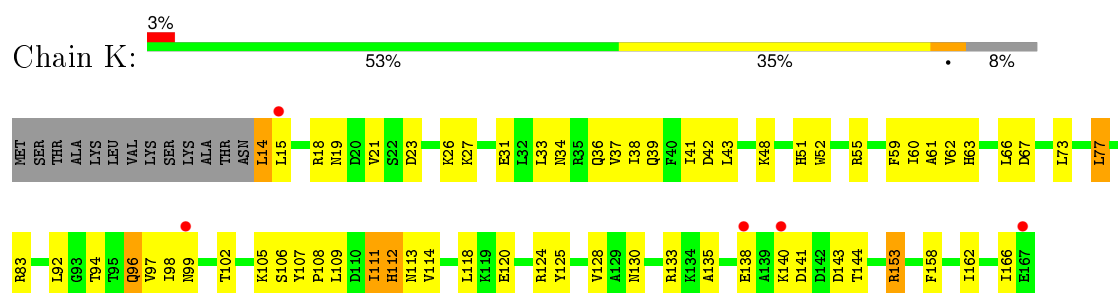
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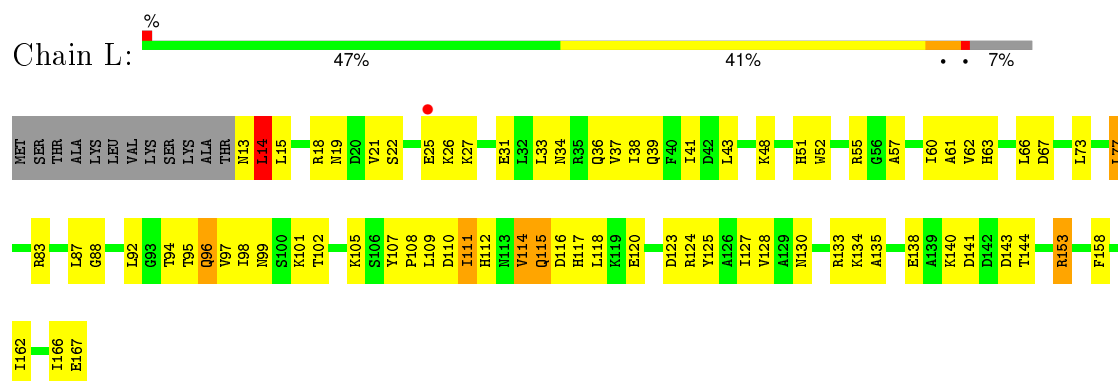
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

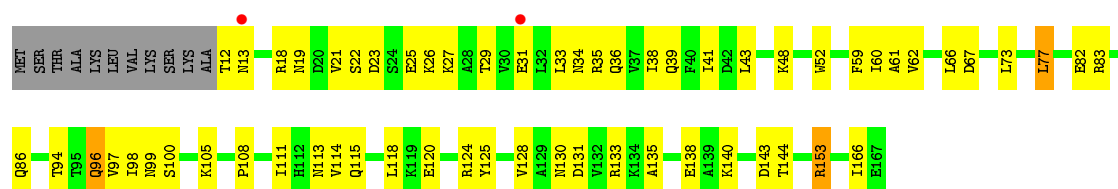


- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

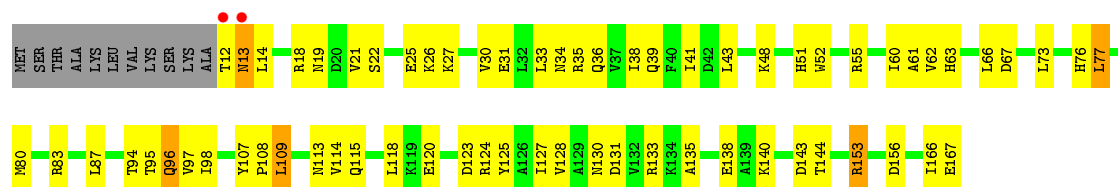


- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

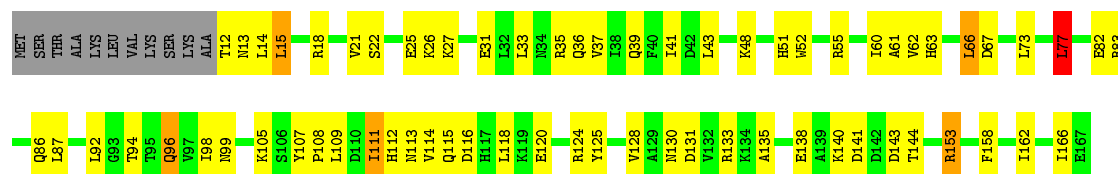




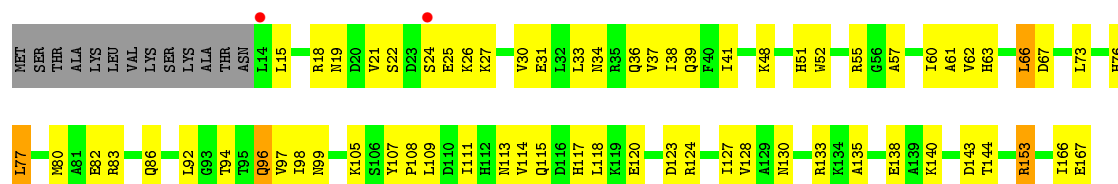
● Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



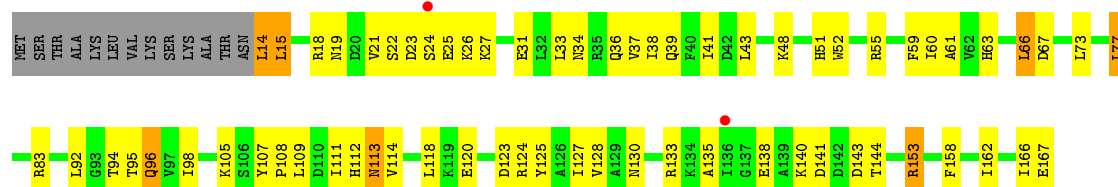
● Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



● Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



● Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



● Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN





T94	T95	Q96	Q98	V97	I98	N99	K105	S106	I107	P108	L109	N113	V114	Q115	D116	H117	L118	K119	E120	R124	V128	A129	N130	R133	K134	A135	E138	A139	K140	D143	T144	R153	F158	I162	I166	E167	T94	T95	Q96	Q98	V97	I98	N99	K105	S106	I107	P108	L109	N113	V114	Q115	D116	H117	L118	K119	E120	R124	V128	A129	N130	R133	K134	A135	E138	A139	K140	D143	T144	R153	F158	I162	I166	E167
MET	SER	THR	ALA	LYS	LEU	VAL	LYS	SER	LYS	ALA	T12	L15	R18	V21	S22	D23	S24	E25	K26	K27	E31	L32	L33	N34	K35	V37	I38	Q39	F40	I41	K48	H51	H52	H55	I60	A61	V62	H63	L66	D67	L73	L77	R83	L87																													

- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

MET	L92	G93	T94	T95	Q96	V97	V98	L99	LYS	K105	S106	P108	ALA	T112	M113	V114	Q115	H116	H117	L118	K119	E120	LYS	E125	K126	LYS	E131	L132	L133	N134	R135	Q136	V137	N138	Q139	F140	D141	L143	LYS	K148	H151	W152	LYS	R155	LYS	I160	A161	V162	H163	L166	D167	LYS	L173	L177	R182
	L93	G94	T95	T96	Q97	V98	V99	K106		S107	P109	T113		M114	Q116	H117	H118	L119	K120	E126	N127	V128		A129	N130		Q131	F132	R133	K134	A135	E138	A139	K140	D141	D142	D143	T144		R153	F158	L159		W160		F161	L162	N165	L166	E167					

- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

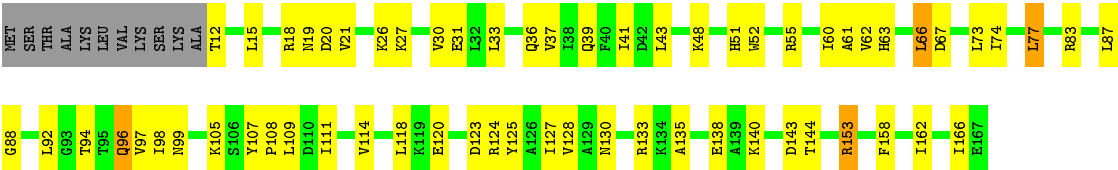
G93	T94	T95	Q96	Y97	I98	M99	T102	K105	I106	Y107	P108	L109	D110	I111	H112	M113	H117	N118	K119	E120	D123	I124	Y125	A126	I127	V128	A129	N130	D131	V132	A133	K134	A135	E138	A139	K140	D143	T144	R153	F158	I162	I166	E167			
SR	SR	THR	ALA	LYS	LEU	VAL	LYS	SR	SR	LYS	T12	M13	L14	R18	M19	D20	V21	S22	D23	K26	K27	E31	I32	I33	N34	Q36	V37	I38	Q39	F40	I41	D42	L43	K48	H51	M52	I60	A61	V62	H63	L66	D67	L73	L77	R83	I93

- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

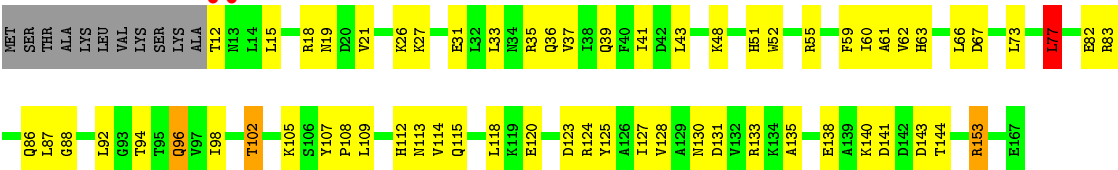
L87	G88		T94	T95	Q96	V97	I98	N99	S100	K101	T102	K105	S106	P107	P108	L109	D110	T111	H112	M113	V114	Q115	L118	K119	E120	R124	V128	A129	M130	D131	V132	R133	K134	A135	E138	A139	K140	D143	T144	R153	F158	I162	I166	E167	L87	G88		T94	T95	Q96	V97	I98	N99	S100	K101	T102	K105	S106	P107	P108	L109	D110	T111	H112	M113	V114	Q115	L118	K119	E120	R124	V128	A129	M130	D131	V132	R133	K134	A135	E138	A139	K140	D143	T144	R153	F158	I162	I166	E167
NET	SER	THR	ALA	LYS	LEU	VAL	LYS	SER	LYS	LYS	ALA	THR	M13	L14	L15	R18	M19	D20	V21	S22	D23	R26	K27	V30	E31	L32	L33	R34	R35	Q36	V37	I38	Q39	F40	I41	K48	H51	W52	R55	V62	H63	L66	D67	L73	L77	R83	R86																																										

- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN





● Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.03Å 91.28Å 164.44Å 96.88° 97.18° 119.86°	Depositor
Resolution (Å)	29.76 – 2.60 29.76 – 2.56	Depositor EDS
% Data completeness (in resolution range)	89.0 (29.76-2.60) 81.5 (29.76-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.57Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.238 , 0.268 0.232 , 0.262	Depositor DCC
R_{free} test set	6021 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.6	EDS
Estimated twinning fraction	0.000 for k,h,-h-k-l 0.000 for -k,-h,-l 0.000 for -h,-k,h+k+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 132451 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29850	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0127e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS

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	0.39	0/1242	0.61	0/1681
1	B	0.41	0/1242	0.60	1/1681 (0.1%)
1	C	0.40	0/1234	0.60	1/1670 (0.1%)
1	D	0.41	0/1234	0.61	0/1670
1	E	0.40	0/1249	0.63	1/1691 (0.1%)
1	F	0.39	0/1242	0.59	0/1681
1	G	0.34	0/1242	0.57	0/1681
1	H	0.37	0/1234	0.58	0/1670
1	I	0.41	0/1234	0.58	0/1670
1	J	0.38	0/1263	0.59	0/1709
1	K	0.38	0/1234	0.57	0/1670
1	L	0.37	0/1242	0.58	0/1681
1	M	0.42	0/1249	0.61	0/1691
1	N	0.44	0/1249	0.61	0/1691
1	O	0.39	0/1249	0.59	1/1691 (0.1%)
1	P	0.40	0/1234	0.59	0/1670
1	Q	0.38	0/1234	0.58	0/1670
1	R	0.40	0/1249	0.58	0/1691
1	S	0.42	0/1249	0.61	1/1691 (0.1%)
1	T	0.47	0/1249	0.66	2/1691 (0.1%)
1	U	0.42	0/1254	0.61	0/1698
1	V	0.45	0/1242	0.62	0/1681
1	W	0.47	0/1249	0.65	0/1691
1	X	0.43	0/1249	0.63	1/1691 (0.1%)
All	All	0.41	0/29848	0.60	8/40402 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	14	LEU	CA-CB-CG	7.37	132.25	115.30
1	E	77	LEU	CA-CB-CG	6.02	129.14	115.30
1	B	77	LEU	CA-CB-CG	5.25	127.37	115.30
1	T	77	LEU	CA-CB-CG	5.21	127.28	115.30
1	X	77	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	77	LEU	CA-CB-CG	5.13	127.11	115.30
1	S	77	LEU	CA-CB-CG	5.12	127.07	115.30
1	O	77	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1224	0	1227	70	0
1	B	1224	0	1227	72	0
1	C	1216	0	1221	63	0
1	D	1216	0	1221	68	0
1	E	1231	0	1234	57	0
1	F	1224	0	1227	53	0
1	G	1224	0	1227	67	0
1	H	1216	0	1221	65	0
1	I	1216	0	1221	53	0
1	J	1245	0	1252	63	0
1	K	1216	0	1221	80	0
1	L	1224	0	1227	81	0
1	M	1231	0	1234	53	0
1	N	1231	0	1234	58	0
1	O	1231	0	1234	71	0
1	P	1216	0	1221	68	0
1	Q	1216	0	1221	68	0
1	R	1231	0	1234	70	0
1	S	1231	0	1234	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1231	0	1234	67	0
1	U	1236	0	1239	67	0
1	V	1224	0	1227	63	0
1	W	1231	0	1234	56	0
1	X	1231	0	1234	56	0
2	A	16	0	24	0	0
2	C	8	0	12	0	0
2	D	24	0	36	0	0
2	E	8	0	12	1	0
2	G	16	0	24	1	0
2	H	16	0	24	0	0
2	L	8	0	12	0	0
2	M	16	0	24	0	0
2	P	24	0	36	1	0
2	Q	8	0	12	1	0
2	R	8	0	12	0	0
2	T	16	0	24	0	0
2	W	16	0	24	0	0
2	X	8	0	12	0	0
3	A	10	0	0	0	0
3	B	8	0	0	1	0
3	C	8	0	0	0	0
3	D	8	0	0	1	0
3	E	10	0	0	1	0
3	F	12	0	0	2	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	8	0	0	2	0
3	J	6	0	0	0	0
3	K	5	0	0	0	0
3	L	8	0	0	1	0
3	M	11	0	0	0	0
3	N	12	0	0	1	0
3	O	11	0	0	0	0
3	P	3	0	0	0	0
3	Q	7	0	0	0	0
3	R	10	0	0	1	0
3	S	11	0	0	0	0
3	T	16	0	0	1	0
3	U	10	0	0	2	0
3	V	11	0	0	2	0
3	W	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	22	0	0	1	0
All	All	29850	0	29794	1452	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 24.

All (1452) 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:R:14:LEU:H	1:R:14:LEU:HD23	1.19	1.02
1:J:12:THR:HA	1:J:27:LYS:NZ	1.75	1.01
1:L:111:ILE:HD11	1:L:116:ASP:HB3	1.45	0.97
1:J:12:THR:HA	1:J:27:LYS:HZ3	1.29	0.95
1:A:109:LEU:HD23	1:B:92:LEU:HD22	1.48	0.94
1:C:109:LEU:HD23	1:D:92:LEU:HD22	1.49	0.94
1:K:92:LEU:HD22	1:L:109:LEU:HD23	1.52	0.92
1:I:99:ASN:HD21	1:J:96:GLN:HA	1.32	0.91
1:W:109:LEU:HD23	1:X:92:LEU:HD22	1.50	0.90
1:U:107:TYR:O	1:U:109:LEU:HD12	1.72	0.89
1:R:14:LEU:H	1:R:14:LEU:CD2	1.85	0.89
1:Q:92:LEU:HD22	1:R:109:LEU:HD23	1.56	0.86
1:D:115:GLN:OE1	1:D:167:GLU:HG2	1.74	0.86
1:O:109:LEU:HD23	1:P:92:LEU:HD22	1.58	0.85
1:A:111:ILE:HD13	1:A:120:GLU:HG3	1.59	0.84
1:O:99:ASN:ND2	1:P:96:GLN:HA	1.93	0.82
1:H:33:LEU:HD21	1:H:144:THR:HG23	1.62	0.81
1:K:18:ARG:HH11	1:K:18:ARG:HG3	1.46	0.81
1:V:33:LEU:HD21	1:V:144:THR:HG23	1.62	0.80
1:P:115:GLN:NE2	1:P:167:GLU:HG2	1.95	0.80
1:K:109:LEU:HD23	1:L:92:LEU:HD22	1.63	0.80
1:I:99:ASN:ND2	1:J:99:ASN:HB3	1.97	0.79
1:W:33:LEU:HD21	1:W:144:THR:HG23	1.64	0.79
1:L:111:ILE:CD1	1:L:116:ASP:HB3	2.10	0.79
1:U:33:LEU:HD21	1:U:144:THR:HG23	1.64	0.79
1:Q:33:LEU:HD21	1:Q:144:THR:HG23	1.64	0.79
1:P:33:LEU:HD21	1:P:144:THR:HG23	1.65	0.79
1:L:115:GLN:NE2	1:L:167:GLU:HG2	1.98	0.78
1:C:33:LEU:HD21	1:C:144:THR:HG23	1.66	0.78
1:T:14:LEU:HD11	1:T:26:LYS:CB	2.13	0.78
1:O:15:LEU:HD23	1:P:55:ARG:HE	1.47	0.78
1:R:21:VAL:O	1:R:26:LYS:HE3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD21	1:A:144:THR:HG23	1.66	0.78
1:S:33:LEU:HD21	1:S:144:THR:HG23	1.66	0.78
1:G:109:LEU:HD23	1:H:92:LEU:HD22	1.66	0.77
1:H:111:ILE:HD12	1:H:116:ASP:HB3	1.66	0.77
1:D:33:LEU:HD21	1:D:144:THR:HG23	1.66	0.77
1:U:92:LEU:HD22	1:V:109:LEU:HD23	1.66	0.77
1:J:41:ILE:HG12	1:J:77:LEU:HD11	1.66	0.77
1:L:33:LEU:HD21	1:L:144:THR:HG23	1.67	0.77
1:J:18:ARG:HH11	1:J:18:ARG:HG3	1.50	0.77
1:B:33:LEU:HD21	1:B:144:THR:HG23	1.68	0.76
1:W:27:LYS:O	1:W:31:GLU:HG2	1.86	0.76
1:T:14:LEU:HD11	1:T:26:LYS:HB2	1.67	0.76
1:W:133:ARG:HB2	1:W:133:ARG:HH11	1.51	0.76
1:F:41:ILE:HG12	1:F:77:LEU:HD11	1.67	0.76
1:C:92:LEU:HD22	1:D:109:LEU:HD23	1.68	0.76
1:D:107:TYR:O	1:D:109:LEU:HD12	1.86	0.75
1:R:55:ARG:O	1:R:114:VAL:HG23	1.84	0.75
1:C:21:VAL:O	1:C:26:LYS:HE3	1.86	0.75
1:X:98:ILE:O	1:X:102:THR:HG22	1.87	0.75
1:E:14:LEU:HD23	1:E:14:LEU:H	1.52	0.75
1:K:33:LEU:HD21	1:K:144:THR:HG23	1.67	0.75
1:L:18:ARG:HG3	1:L:18:ARG:HH11	1.52	0.75
1:J:10:LYS:HG3	1:J:11:ALA:H	1.50	0.75
1:V:94:THR:HB	1:V:96:GLN:HE21	1.49	0.75
1:K:94:THR:HB	1:K:96:GLN:HE21	1.52	0.75
1:P:25:GLU:OE1	1:P:140:LYS:HB2	1.87	0.74
1:I:99:ASN:ND2	1:J:96:GLN:HA	2.02	0.74
1:X:33:LEU:HD21	1:X:144:THR:HG23	1.70	0.74
1:P:27:LYS:O	1:P:31:GLU:HG2	1.88	0.74
1:G:18:ARG:HG3	1:G:18:ARG:HH11	1.52	0.74
1:K:105:LYS:HE2	1:K:124:ARG:NH1	2.03	0.74
1:Q:41:ILE:HG12	1:Q:77:LEU:HD11	1.68	0.73
1:J:27:LYS:O	1:J:31:GLU:HG2	1.87	0.73
1:M:27:LYS:O	1:M:31:GLU:HG2	1.88	0.73
1:E:33:LEU:HD21	1:E:144:THR:HG23	1.70	0.73
1:L:27:LYS:O	1:L:31:GLU:HG2	1.89	0.73
1:F:33:LEU:HD21	1:F:144:THR:HG23	1.70	0.73
1:F:27:LYS:O	1:F:31:GLU:HG2	1.88	0.73
1:D:27:LYS:O	1:D:31:GLU:HG2	1.88	0.73
1:J:33:LEU:HD21	1:J:144:THR:HG23	1.70	0.73
1:R:33:LEU:HD21	1:R:144:THR:HG23	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:94:THR:HB	1:Q:96:GLN:HE21	1.52	0.73
1:U:27:LYS:O	1:U:31:GLU:HG2	1.88	0.73
1:V:27:LYS:O	1:V:31:GLU:HG2	1.89	0.73
1:R:27:LYS:O	1:R:31:GLU:HG2	1.89	0.73
1:P:18:ARG:HG3	1:P:18:ARG:HH11	1.54	0.73
1:K:41:ILE:HG12	1:K:77:LEU:HD11	1.70	0.73
1:V:21:VAL:O	1:V:26:LYS:HE3	1.89	0.73
1:X:21:VAL:O	1:X:26:LYS:HE3	1.89	0.72
1:N:153:ARG:HH11	1:N:153:ARG:HG2	1.53	0.72
1:S:27:LYS:O	1:S:31:GLU:HG2	1.89	0.72
1:H:27:LYS:O	1:H:31:GLU:HG2	1.89	0.72
1:D:18:ARG:HG3	1:D:18:ARG:HH11	1.54	0.72
1:I:41:ILE:HG12	1:I:77:LEU:HD11	1.69	0.72
1:W:55:ARG:O	1:W:114:VAL:HG23	1.90	0.72
1:L:94:THR:HB	1:L:96:GLN:HE21	1.54	0.72
1:X:107:TYR:O	1:X:109:LEU:HD12	1.89	0.72
1:G:33:LEU:HD21	1:G:144:THR:HG23	1.71	0.72
1:Q:133:ARG:HH11	1:Q:133:ARG:HB2	1.54	0.72
1:G:27:LYS:O	1:G:31:GLU:HG2	1.90	0.72
1:D:133:ARG:HH11	1:D:133:ARG:HB2	1.55	0.72
1:G:55:ARG:O	1:G:114:VAL:HG23	1.89	0.72
1:L:115:GLN:HE22	1:L:167:GLU:H	1.35	0.72
1:S:99:ASN:HB2	1:T:95:THR:HG22	1.71	0.72
1:K:27:LYS:O	1:K:31:GLU:HG2	1.89	0.72
1:F:18:ARG:HG3	1:F:18:ARG:HH11	1.55	0.72
1:D:94:THR:HB	1:D:96:GLN:HE21	1.55	0.72
1:A:21:VAL:O	1:A:26:LYS:HE3	1.90	0.71
1:E:153:ARG:HH11	1:E:153:ARG:HG2	1.54	0.71
1:U:18:ARG:HH11	1:U:18:ARG:HG3	1.55	0.71
1:D:115:GLN:HA	1:D:115:GLN:HE21	1.56	0.71
1:D:41:ILE:HG12	1:D:77:LEU:HD11	1.71	0.71
1:G:41:ILE:HG12	1:G:77:LEU:HD11	1.73	0.71
1:A:107:TYR:O	1:A:109:LEU:HD12	1.90	0.71
1:R:18:ARG:HG3	1:R:18:ARG:HH11	1.54	0.71
1:D:21:VAL:O	1:D:26:LYS:HE3	1.90	0.71
1:I:27:LYS:O	1:I:31:GLU:HG2	1.91	0.71
1:P:94:THR:HB	1:P:96:GLN:HE21	1.56	0.71
1:H:94:THR:HB	1:H:96:GLN:HE21	1.54	0.71
1:U:133:ARG:HH11	1:U:133:ARG:HB2	1.55	0.71
1:M:33:LEU:HD21	1:M:144:THR:HG23	1.73	0.71
1:P:21:VAL:O	1:P:26:LYS:HE3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:LYS:O	1:E:31:GLU:HG2	1.91	0.71
1:T:18:ARG:HH11	1:T:18:ARG:HG3	1.54	0.71
1:Q:27:LYS:O	1:Q:31:GLU:HG2	1.90	0.70
1:K:108:PRO:HB2	1:K:111:ILE:HG12	1.73	0.70
1:B:94:THR:HB	1:B:96:GLN:HE21	1.56	0.70
1:S:94:THR:HB	1:S:96:GLN:HE21	1.56	0.70
1:G:94:THR:HB	1:G:96:GLN:HE21	1.57	0.70
1:E:99:ASN:HB3	1:F:99:ASN:HD22	1.56	0.70
1:B:55:ARG:O	1:B:114:VAL:HG23	1.92	0.70
1:H:21:VAL:O	1:H:26:LYS:HE3	1.91	0.70
1:I:33:LEU:HD21	1:I:144:THR:HG23	1.72	0.70
1:L:133:ARG:HB2	1:L:133:ARG:HH11	1.57	0.70
1:U:92:LEU:CD2	1:V:109:LEU:HD23	2.21	0.70
1:W:94:THR:HB	1:W:96:GLN:HE21	1.57	0.70
1:S:95:THR:HG22	1:T:99:ASN:HB2	1.73	0.69
1:W:107:TYR:O	1:W:109:LEU:HD12	1.90	0.69
1:E:14:LEU:H	1:E:14:LEU:CD2	2.05	0.69
1:S:21:VAL:O	1:S:26:LYS:HE3	1.92	0.69
1:S:41:ILE:HG12	1:S:77:LEU:HD11	1.74	0.69
1:Q:18:ARG:HH11	1:Q:18:ARG:HG3	1.56	0.69
1:D:36:GLN:HA	1:D:36:GLN:HE21	1.57	0.69
1:V:35:ARG:HD3	3:V:696:HOH:O	1.91	0.69
1:Q:21:VAL:O	1:Q:26:LYS:HE3	1.92	0.69
1:B:27:LYS:O	1:B:31:GLU:HG2	1.93	0.69
1:S:18:ARG:HG3	1:S:18:ARG:HH11	1.58	0.69
1:O:27:LYS:O	1:O:31:GLU:HG2	1.92	0.69
1:E:18:ARG:HG3	1:E:18:ARG:HH11	1.57	0.69
1:R:41:ILE:HG12	1:R:77:LEU:HD11	1.74	0.68
1:B:133:ARG:HB2	1:B:133:ARG:HH11	1.58	0.68
1:L:22:SER:OG	1:L:25:GLU:HB2	1.94	0.68
1:I:21:VAL:O	1:I:26:LYS:HE3	1.94	0.68
1:C:113:ASN:O	1:C:116:ASP:HB2	1.93	0.68
1:J:21:VAL:O	1:J:26:LYS:HE3	1.93	0.68
1:O:33:LEU:HD21	1:O:144:THR:HG23	1.74	0.68
1:J:12:THR:HA	1:J:27:LYS:CE	2.24	0.68
1:R:94:THR:HB	1:R:96:GLN:HE21	1.59	0.68
1:T:21:VAL:O	1:T:26:LYS:HE3	1.93	0.67
1:U:133:ARG:NH1	1:U:133:ARG:HB2	2.09	0.67
1:T:27:LYS:O	1:T:31:GLU:HG2	1.93	0.67
1:V:18:ARG:HH11	1:V:18:ARG:HG3	1.59	0.67
1:W:21:VAL:O	1:W:26:LYS:HE3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:133:ARG:HB2	1:W:133:ARG:NH1	2.08	0.67
1:A:15:LEU:HD23	1:A:88:GLY:O	1.94	0.67
1:O:133:ARG:HH11	1:O:133:ARG:HB2	1.59	0.67
1:A:27:LYS:O	1:A:31:GLU:HG2	1.93	0.67
1:M:41:ILE:HG12	1:M:77:LEU:HD11	1.76	0.67
1:N:94:THR:HB	1:N:96:GLN:HE21	1.58	0.67
1:M:18:ARG:HG3	1:M:18:ARG:HH11	1.59	0.67
1:K:105:LYS:HE2	1:K:124:ARG:HH12	1.58	0.67
1:G:13:ASN:HB3	1:G:27:LYS:HE2	1.76	0.67
1:O:41:ILE:HG12	1:O:77:LEU:HD11	1.76	0.67
1:J:94:THR:HB	1:J:96:GLN:HE21	1.59	0.67
1:Q:133:ARG:HB2	1:Q:133:ARG:NH1	2.10	0.67
1:E:105:LYS:O	1:E:124:ARG:NH1	2.28	0.67
1:C:111:ILE:CD1	1:C:120:GLU:HG3	2.25	0.67
1:A:37:VAL:O	1:A:41:ILE:HG13	1.95	0.67
1:N:27:LYS:O	1:N:31:GLU:HG2	1.95	0.67
1:D:133:ARG:HB2	1:D:133:ARG:NH1	2.10	0.67
1:X:27:LYS:O	1:X:31:GLU:HG2	1.93	0.67
1:F:21:VAL:O	1:F:26:LYS:HE3	1.94	0.67
1:S:133:ARG:NH1	1:S:133:ARG:HB2	2.10	0.67
1:X:18:ARG:HH11	1:X:18:ARG:HG3	1.58	0.67
1:X:94:THR:HB	1:X:96:GLN:HE21	1.60	0.66
1:T:94:THR:HB	1:T:96:GLN:HE21	1.61	0.66
1:P:133:ARG:HB2	1:P:133:ARG:HH11	1.60	0.66
1:J:133:ARG:HH11	1:J:133:ARG:HB2	1.61	0.66
1:S:133:ARG:HH11	1:S:133:ARG:HB2	1.61	0.66
1:I:18:ARG:HG3	1:I:18:ARG:HH11	1.59	0.66
1:U:94:THR:HB	1:U:96:GLN:HE21	1.60	0.66
1:C:27:LYS:O	1:C:31:GLU:HG2	1.95	0.66
1:N:18:ARG:HG3	1:N:18:ARG:HH11	1.60	0.66
1:C:107:TYR:O	1:C:109:LEU:HD12	1.95	0.66
1:N:153:ARG:HG2	1:N:153:ARG:NH1	2.09	0.66
1:K:133:ARG:HH11	1:K:133:ARG:HB2	1.60	0.66
1:L:107:TYR:O	1:L:109:LEU:HD12	1.94	0.66
1:F:22:SER:OG	1:F:25:GLU:HB2	1.96	0.66
1:N:33:LEU:HD21	1:N:144:THR:HG23	1.77	0.66
1:L:108:PRO:HB2	1:L:111:ILE:HG22	1.77	0.66
1:M:94:THR:HB	1:M:96:GLN:HE21	1.61	0.66
1:A:41:ILE:HG12	1:A:77:LEU:HD11	1.76	0.65
1:N:21:VAL:O	1:N:26:LYS:HE3	1.96	0.65
1:Q:92:LEU:CD2	1:R:109:LEU:HD23	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:LEU:HD12	1:E:109:LEU:H	1.62	0.65
1:E:94:THR:HB	1:E:96:GLN:HE21	1.61	0.65
1:G:133:ARG:HB2	1:G:133:ARG:HH11	1.60	0.65
1:O:133:ARG:NH1	1:O:133:ARG:HB2	2.12	0.65
1:Q:109:LEU:HD23	1:R:92:LEU:HD22	1.79	0.65
1:M:133:ARG:NH1	1:M:133:ARG:HB2	2.11	0.65
1:B:107:TYR:O	1:B:109:LEU:HD12	1.97	0.65
1:L:133:ARG:HB2	1:L:133:ARG:NH1	2.12	0.65
1:L:105:LYS:O	1:L:124:ARG:NH1	2.30	0.65
1:U:41:ILE:HG12	1:U:77:LEU:HD11	1.78	0.65
1:E:153:ARG:HG2	1:E:153:ARG:NH1	2.11	0.64
1:A:94:THR:HB	1:A:96:GLN:HE21	1.62	0.64
1:G:107:TYR:O	1:G:109:LEU:HD12	1.98	0.64
1:C:41:ILE:HG12	1:C:77:LEU:HD11	1.79	0.64
1:G:21:VAL:O	1:G:26:LYS:HE3	1.96	0.64
1:A:99:ASN:HB3	1:B:95:THR:HG22	1.77	0.64
1:C:55:ARG:O	1:C:114:VAL:HG23	1.97	0.64
1:C:133:ARG:HB2	1:C:133:ARG:HH11	1.63	0.64
1:P:108:PRO:HB2	1:P:111:ILE:HG12	1.79	0.64
1:V:153:ARG:HG3	3:V:655:HOH:O	1.98	0.64
1:T:41:ILE:HG12	1:T:77:LEU:HD11	1.79	0.64
1:O:107:TYR:O	1:O:109:LEU:HD12	1.98	0.64
1:L:41:ILE:HG12	1:L:77:LEU:HD11	1.80	0.64
1:T:111:ILE:HG13	1:T:117:HIS:CE1	2.33	0.64
1:K:99:ASN:HB3	1:L:99:ASN:HD22	1.62	0.64
1:F:107:TYR:O	1:F:109:LEU:HD13	1.98	0.64
1:K:108:PRO:HB2	1:K:111:ILE:CG1	2.27	0.64
1:P:41:ILE:HG12	1:P:77:LEU:HD11	1.80	0.64
1:T:14:LEU:HD21	1:T:26:LYS:HD3	1.80	0.64
1:U:21:VAL:O	1:U:26:LYS:HE3	1.96	0.64
1:V:15:LEU:HD23	1:V:88:GLY:O	1.98	0.64
1:L:108:PRO:HB2	1:L:111:ILE:CG2	2.28	0.63
1:L:111:ILE:CG1	1:L:116:ASP:HB3	2.28	0.63
1:P:133:ARG:HB2	1:P:133:ARG:NH1	2.14	0.63
1:I:94:THR:HB	1:I:96:GLN:HE21	1.62	0.63
1:B:41:ILE:HG12	1:B:77:LEU:HD11	1.78	0.63
1:G:99:ASN:HB3	1:H:99:ASN:ND2	2.14	0.63
1:X:133:ARG:HH11	1:X:133:ARG:HB2	1.62	0.63
1:H:41:ILE:HG12	1:H:77:LEU:HD11	1.79	0.63
1:V:55:ARG:O	1:V:114:VAL:HG23	1.98	0.63
1:B:133:ARG:HB2	1:B:133:ARG:NH1	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:133:ARG:HB2	1:V:133:ARG:HH11	1.64	0.63
1:Q:15:LEU:HD21	1:R:112:HIS:NE2	2.13	0.63
1:B:18:ARG:HG3	1:B:18:ARG:HH11	1.63	0.63
1:K:99:ASN:CB	1:L:99:ASN:HD22	2.11	0.63
1:N:41:ILE:HG12	1:N:77:LEU:HD11	1.81	0.63
1:M:133:ARG:HH11	1:M:133:ARG:HB2	1.63	0.63
1:K:18:ARG:HG3	1:K:18:ARG:NH1	2.14	0.63
1:E:99:ASN:HB2	1:F:95:THR:HG22	1.81	0.63
1:A:18:ARG:HG3	1:A:18:ARG:HH11	1.63	0.63
1:J:133:ARG:NH1	1:J:133:ARG:HB2	2.14	0.62
1:E:99:ASN:HB3	1:F:99:ASN:ND2	2.14	0.62
1:S:115:GLN:HE22	1:S:166:ILE:HA	1.64	0.62
1:B:48:LYS:HD2	1:B:52:TRP:CE2	2.34	0.62
1:A:153:ARG:HH11	1:A:153:ARG:HG2	1.64	0.62
1:T:33:LEU:HD21	1:T:144:THR:HG23	1.80	0.62
1:U:92:LEU:HD22	1:V:109:LEU:CD2	2.29	0.62
1:B:21:VAL:O	1:B:26:LYS:HE3	1.99	0.62
1:X:41:ILE:HG12	1:X:77:LEU:HD11	1.82	0.62
1:I:105:LYS:O	1:I:124:ARG:NH1	2.33	0.62
1:O:92:LEU:HD22	1:P:109:LEU:HD23	1.82	0.62
1:M:21:VAL:O	1:M:26:LYS:HE3	2.00	0.62
1:H:18:ARG:HG3	1:H:18:ARG:HH11	1.65	0.62
1:K:21:VAL:O	1:K:26:LYS:HE3	1.99	0.62
1:G:99:ASN:CB	1:H:99:ASN:HD22	2.12	0.62
1:E:109:LEU:N	1:E:109:LEU:HD12	2.14	0.62
1:E:21:VAL:O	1:E:26:LYS:HE3	1.98	0.61
1:H:153:ARG:HG2	1:H:153:ARG:HH11	1.65	0.61
1:O:18:ARG:HG3	1:O:18:ARG:HH11	1.64	0.61
1:O:105:LYS:O	1:O:124:ARG:NH1	2.33	0.61
1:K:108:PRO:HB2	1:K:111:ILE:CD1	2.28	0.61
1:D:94:THR:O	1:D:98:ILE:HG12	2.00	0.61
1:W:41:ILE:HG12	1:W:77:LEU:HD11	1.80	0.61
1:K:133:ARG:HB2	1:K:133:ARG:NH1	2.14	0.61
1:C:48:LYS:HD2	1:C:52:TRP:CE2	2.35	0.61
1:L:15:LEU:HD23	1:L:88:GLY:O	2.01	0.61
1:J:18:ARG:HG3	1:J:18:ARG:NH1	2.16	0.61
1:K:105:LYS:NZ	1:K:124:ARG:HH22	1.99	0.61
1:D:22:SER:OG	1:D:25:GLU:HB2	2.01	0.61
1:Q:96:GLN:HA	1:R:99:ASN:HD22	1.66	0.61
1:Q:14:LEU:HD23	1:Q:14:LEU:N	2.15	0.61
1:O:94:THR:HB	1:O:96:GLN:HE21	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:153:ARG:HH11	1:O:153:ARG:HG2	1.65	0.61
1:G:133:ARG:HB2	1:G:133:ARG:NH1	2.15	0.61
1:C:109:LEU:HD12	1:C:109:LEU:N	2.16	0.60
1:K:109:LEU:HD12	1:K:109:LEU:N	2.16	0.60
1:J:48:LYS:HD2	1:J:52:TRP:CE2	2.35	0.60
1:F:94:THR:HB	1:F:96:GLN:HE21	1.66	0.60
1:W:18:ARG:HG3	1:W:18:ARG:HH11	1.65	0.60
1:V:41:ILE:HG12	1:V:77:LEU:HD11	1.82	0.60
1:F:48:LYS:HD2	1:F:52:TRP:CE2	2.35	0.60
1:V:36:GLN:HE21	1:V:36:GLN:HA	1.66	0.60
1:H:55:ARG:O	1:H:114:VAL:HG23	2.00	0.60
1:P:48:LYS:HD2	1:P:52:TRP:CE2	2.36	0.60
1:S:48:LYS:HD2	1:S:52:TRP:CE2	2.37	0.60
1:J:15:LEU:HD23	1:J:88:GLY:O	2.02	0.60
1:X:133:ARG:NH1	1:X:133:ARG:HB2	2.16	0.60
1:D:48:LYS:HD2	1:D:52:TRP:CE2	2.36	0.60
1:D:55:ARG:O	1:D:114:VAL:HG23	2.01	0.60
1:I:109:LEU:HD23	1:J:92:LEU:HD22	1.83	0.60
1:E:133:ARG:HB2	1:E:133:ARG:NH1	2.16	0.60
1:W:109:LEU:HD23	1:X:92:LEU:CD2	2.28	0.60
1:D:36:GLN:HA	1:D:36:GLN:NE2	2.16	0.60
1:R:14:LEU:N	1:R:14:LEU:HD23	2.03	0.60
1:D:113:ASN:OD1	1:D:115:GLN:N	2.35	0.60
1:F:77:LEU:HD23	1:F:77:LEU:C	2.22	0.60
1:K:111:ILE:HD13	1:K:120:GLU:HG3	1.84	0.60
1:F:55:ARG:O	1:F:114:VAL:HG23	2.02	0.60
1:Q:95:THR:HG22	1:R:99:ASN:HB2	1.84	0.60
1:W:92:LEU:HD22	1:X:109:LEU:HD23	1.83	0.60
1:A:153:ARG:NH1	1:A:153:ARG:HG2	2.16	0.60
1:Q:83:ARG:NH2	1:Q:143:ASP:HB2	2.16	0.60
1:P:113:ASN:OD1	1:P:115:GLN:HB2	2.00	0.60
1:G:18:ARG:NH1	1:G:18:ARG:HG3	2.16	0.60
1:W:15:LEU:HD23	1:W:88:GLY:O	2.02	0.60
1:S:107:TYR:O	1:S:109:LEU:HD12	2.02	0.60
1:M:105:LYS:HE2	1:M:124:ARG:NH2	2.16	0.59
1:G:99:ASN:HB3	1:H:99:ASN:HD22	1.67	0.59
1:M:105:LYS:O	1:M:124:ARG:NH1	2.35	0.59
1:T:18:ARG:HG3	1:T:18:ARG:NH1	2.18	0.59
1:L:115:GLN:NE2	1:L:167:GLU:H	2.00	0.59
1:A:97:VAL:CG2	1:B:109:LEU:HD21	2.31	0.59
1:A:48:LYS:HD2	1:A:52:TRP:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:96:GLN:HA	1:L:99:ASN:ND2	2.17	0.59
1:Q:36:GLN:HE21	1:Q:36:GLN:HA	1.67	0.59
1:S:99:ASN:HD22	1:T:96:GLN:HA	1.68	0.59
1:C:15:LEU:HD11	1:D:112:HIS:CD2	2.37	0.59
1:A:133:ARG:HB2	1:A:133:ARG:HH11	1.66	0.59
1:E:133:ARG:HB2	1:E:133:ARG:HH11	1.67	0.59
1:S:94:THR:O	1:S:98:ILE:HG12	2.02	0.59
1:V:133:ARG:HB2	1:V:133:ARG:NH1	2.17	0.59
1:W:153:ARG:HG2	1:W:153:ARG:HH11	1.68	0.59
1:K:94:THR:O	1:K:98:ILE:HG12	2.02	0.59
1:W:94:THR:O	1:W:98:ILE:HG12	2.03	0.59
1:A:98:ILE:O	1:A:102:THR:HG22	2.02	0.59
1:I:36:GLN:NE2	1:I:36:GLN:HA	2.18	0.59
1:L:111:ILE:HD11	1:L:116:ASP:C	2.22	0.58
1:O:99:ASN:HD21	1:P:96:GLN:HA	1.68	0.58
1:K:48:LYS:HD2	1:K:52:TRP:CE2	2.38	0.58
1:C:133:ARG:HB2	1:C:133:ARG:NH1	2.17	0.58
1:E:55:ARG:O	1:E:114:VAL:HG23	2.03	0.58
1:F:114:VAL:O	1:F:118:LEU:HD13	2.04	0.58
1:U:105:LYS:HG2	1:U:106:SER:N	2.18	0.58
1:C:94:THR:HB	1:C:96:GLN:HE21	1.66	0.58
1:R:14:LEU:N	1:R:14:LEU:CD2	2.60	0.58
1:O:153:ARG:HG2	1:O:153:ARG:NH1	2.18	0.58
1:H:105:LYS:O	1:H:124:ARG:NH1	2.37	0.58
1:Q:48:LYS:HD2	1:Q:52:TRP:CE2	2.39	0.58
1:M:48:LYS:HD2	1:M:52:TRP:CE2	2.38	0.58
1:W:36:GLN:HA	1:W:36:GLN:HE21	1.67	0.58
1:U:18:ARG:HG3	1:U:18:ARG:NH1	2.18	0.58
1:X:12:THR:O	1:X:27:LYS:HE2	2.04	0.58
1:H:153:ARG:NH1	1:H:153:ARG:HG2	2.18	0.58
1:G:14:LEU:H	1:G:14:LEU:HD23	1.68	0.58
1:G:120:GLU:O	1:G:124:ARG:HG2	2.04	0.58
1:K:108:PRO:HB2	1:K:111:ILE:HD11	1.84	0.58
1:V:36:GLN:NE2	1:V:36:GLN:HA	2.17	0.58
1:A:133:ARG:HB2	1:A:133:ARG:NH1	2.18	0.58
1:J:105:LYS:O	1:J:124:ARG:NH1	2.36	0.58
1:B:94:THR:O	1:B:98:ILE:HG12	2.04	0.58
1:O:111:ILE:O	1:O:112:HIS:ND1	2.36	0.58
1:K:105:LYS:HE3	1:K:106:SER:O	2.04	0.58
1:B:114:VAL:O	1:B:118:LEU:HD13	2.04	0.58
1:O:22:SER:OG	1:O:25:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:21:VAL:O	1:O:26:LYS:HE3	2.03	0.58
1:T:105:LYS:O	1:T:124:ARG:NH1	2.36	0.58
1:A:109:LEU:HD23	1:B:92:LEU:CD2	2.29	0.58
1:I:99:ASN:HD22	1:J:99:ASN:HB3	1.68	0.58
1:D:115:GLN:CA	1:D:115:GLN:HE21	2.13	0.58
1:T:94:THR:O	1:T:98:ILE:HG12	2.04	0.57
1:R:18:ARG:NH1	1:R:18:ARG:HG3	2.19	0.57
1:M:99:ASN:HD22	1:N:96:GLN:HA	1.69	0.57
1:J:113:ASN:OD1	1:J:115:GLN:N	2.37	0.57
1:N:153:ARG:CG	1:N:153:ARG:HH11	2.17	0.57
1:Q:107:TYR:O	1:Q:109:LEU:HD12	2.04	0.57
1:M:36:GLN:HE21	1:M:36:GLN:HA	1.68	0.57
1:A:111:ILE:HG13	1:A:117:HIS:CE1	2.39	0.57
1:B:37:VAL:O	1:B:41:ILE:HG13	2.05	0.57
1:O:48:LYS:HD2	1:O:52:TRP:CE2	2.39	0.57
1:G:153:ARG:HG2	1:G:153:ARG:HH11	1.70	0.57
1:F:18:ARG:NH1	1:F:18:ARG:HG3	2.19	0.57
1:R:48:LYS:HD2	1:R:52:TRP:CE2	2.40	0.57
1:A:96:GLN:HA	1:B:99:ASN:HD22	1.69	0.57
1:L:18:ARG:NH1	1:L:18:ARG:HG3	2.18	0.57
1:L:120:GLU:O	1:L:124:ARG:HG2	2.05	0.57
1:R:55:ARG:C	1:R:114:VAL:HG23	2.24	0.57
1:G:153:ARG:HG2	1:G:153:ARG:NH1	2.19	0.57
1:H:133:ARG:HH11	1:H:133:ARG:HB2	1.69	0.57
1:Q:51:HIS:O	1:Q:63:HIS:HD2	1.88	0.57
1:V:109:LEU:N	1:V:109:LEU:HD12	2.19	0.56
1:C:54:MET:HB2	1:C:114:VAL:HG22	1.87	0.56
1:L:21:VAL:O	1:L:26:LYS:HE3	2.05	0.56
1:C:153:ARG:NH1	1:C:153:ARG:HG2	2.20	0.56
1:L:48:LYS:HE3	3:L:731:HOH:O	2.05	0.56
1:S:15:LEU:HD23	1:T:55:ARG:HE	1.70	0.56
1:C:109:LEU:HD23	1:D:92:LEU:CD2	2.29	0.56
1:V:98:ILE:O	1:V:102:THR:HG22	2.04	0.56
1:P:18:ARG:HG3	1:P:18:ARG:NH1	2.18	0.56
1:X:37:VAL:O	1:X:41:ILE:HG13	2.05	0.56
1:X:48:LYS:HD2	1:X:52:TRP:CE2	2.40	0.56
1:U:48:LYS:HD2	1:U:52:TRP:CE2	2.40	0.56
1:M:94:THR:O	1:M:98:ILE:HG12	2.05	0.56
1:W:153:ARG:HG2	1:W:153:ARG:NH1	2.20	0.56
1:W:36:GLN:HA	1:W:36:GLN:NE2	2.21	0.56
1:J:99:ASN:O	1:J:102:THR:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:153:ARG:HG3	3:N:591:HOH:O	2.06	0.56
1:D:18:ARG:HG3	1:D:18:ARG:NH1	2.19	0.56
1:F:94:THR:O	1:F:98:ILE:HG12	2.05	0.56
1:Q:60:ILE:HG23	1:Q:61:ALA:N	2.20	0.56
1:F:123:ASP:O	1:F:127:ILE:HD13	2.06	0.56
1:Q:94:THR:O	1:Q:98:ILE:HG12	2.05	0.56
1:H:48:LYS:HD2	1:H:52:TRP:CE2	2.41	0.56
1:H:133:ARG:HB2	1:H:133:ARG:NH1	2.21	0.56
1:I:18:ARG:NH1	1:I:18:ARG:HG3	2.21	0.56
1:X:43:LEU:HD11	1:X:125:TYR:CD1	2.41	0.56
1:M:153:ARG:HH11	1:M:153:ARG:HG2	1.71	0.56
1:Q:36:GLN:NE2	1:Q:36:GLN:HA	2.21	0.56
1:H:14:LEU:HD11	1:H:27:LYS:HG3	1.87	0.55
1:U:94:THR:O	1:U:98:ILE:HG12	2.05	0.55
1:U:120:GLU:O	1:U:124:ARG:HG2	2.06	0.55
1:E:43:LEU:HD11	1:E:125:TYR:CD1	2.40	0.55
1:R:133:ARG:HB2	1:R:133:ARG:NH1	2.19	0.55
1:A:48:LYS:HE3	3:B:746:HOH:O	2.04	0.55
1:M:36:GLN:NE2	1:M:36:GLN:HA	2.21	0.55
1:X:94:THR:O	1:X:98:ILE:HG12	2.06	0.55
1:V:48:LYS:HD2	1:V:52:TRP:CE2	2.41	0.55
1:V:105:LYS:O	1:V:124:ARG:NH1	2.39	0.55
1:L:94:THR:O	1:L:98:ILE:HG12	2.05	0.55
1:L:98:ILE:O	1:L:102:THR:HG22	2.05	0.55
1:L:48:LYS:HD2	1:L:52:TRP:CE2	2.42	0.55
1:U:13:ASN:H	1:U:27:LYS:HE2	1.70	0.55
1:B:98:ILE:O	1:B:102:THR:HG22	2.06	0.55
1:N:18:ARG:HG3	1:N:18:ARG:NH1	2.22	0.55
1:T:51:HIS:O	1:T:63:HIS:HD2	1.89	0.55
1:V:26:LYS:HD3	1:V:87:LEU:O	2.07	0.55
1:C:153:ARG:HH11	1:C:153:ARG:HG2	1.71	0.55
1:C:36:GLN:HE21	1:C:36:GLN:HA	1.72	0.55
1:G:99:ASN:CB	1:H:99:ASN:ND2	2.69	0.55
1:Q:18:ARG:NH1	1:Q:18:ARG:HG3	2.22	0.55
1:L:60:ILE:HG23	1:L:61:ALA:N	2.21	0.55
1:V:62:VAL:HG11	1:V:118:LEU:HD11	1.88	0.55
1:R:36:GLN:NE2	1:R:36:GLN:HA	2.22	0.55
1:B:15:LEU:N	1:B:15:LEU:HD12	2.22	0.55
1:C:37:VAL:O	1:C:41:ILE:HG13	2.06	0.55
1:X:48:LYS:HE3	3:X:657:HOH:O	2.06	0.55
1:H:83:ARG:NH2	1:H:143:ASP:HB2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:111:ILE:O	1:M:111:ILE:HG13	2.07	0.55
1:K:109:LEU:HD23	1:L:92:LEU:CD2	2.35	0.55
1:J:77:LEU:HD23	1:J:77:LEU:C	2.28	0.55
1:V:13:ASN:HB3	1:V:27:LYS:HE2	1.89	0.55
1:G:83:ARG:NH2	1:G:143:ASP:HB2	2.22	0.55
1:G:99:ASN:ND2	1:H:96:GLN:HA	2.22	0.55
1:C:120:GLU:O	1:C:124:ARG:HG2	2.08	0.55
1:I:36:GLN:HE21	1:I:36:GLN:HA	1.72	0.55
1:G:15:LEU:HD22	1:G:15:LEU:N	2.22	0.55
1:L:57:ALA:O	1:L:114:VAL:HG21	2.06	0.55
1:B:153:ARG:HG2	1:B:153:ARG:NH1	2.22	0.55
1:B:36:GLN:HA	1:B:36:GLN:NE2	2.22	0.55
1:J:153:ARG:HG2	1:J:153:ARG:HH11	1.72	0.55
1:J:153:ARG:HG2	1:J:153:ARG:NH1	2.22	0.55
1:Q:111:ILE:CD1	1:Q:120:GLU:HG3	2.37	0.54
1:K:39:GLN:HG2	1:K:128:VAL:HG22	1.89	0.54
1:Q:96:GLN:HA	1:R:99:ASN:ND2	2.22	0.54
1:E:18:ARG:HG3	1:E:18:ARG:NH1	2.21	0.54
1:V:37:VAL:O	1:V:41:ILE:HG13	2.07	0.54
1:E:41:ILE:HG12	1:E:77:LEU:HD11	1.90	0.54
1:A:105:LYS:O	1:A:124:ARG:NH1	2.40	0.54
1:K:120:GLU:O	1:K:124:ARG:HG2	2.07	0.54
1:O:94:THR:O	1:O:98:ILE:HG12	2.08	0.54
1:H:94:THR:O	1:H:98:ILE:HG12	2.07	0.54
1:N:94:THR:O	1:N:98:ILE:HG12	2.07	0.54
1:J:120:GLU:O	1:J:124:ARG:HG2	2.08	0.54
1:I:77:LEU:C	1:I:77:LEU:HD23	2.28	0.54
1:E:153:ARG:HH11	1:E:153:ARG:CG	2.19	0.54
1:U:43:LEU:HD11	1:U:125:TYR:CD1	2.43	0.54
1:M:113:ASN:OD1	1:M:115:GLN:N	2.40	0.54
1:N:39:GLN:HG2	1:N:128:VAL:HG22	1.88	0.54
1:R:37:VAL:O	1:R:41:ILE:HG13	2.07	0.54
1:B:36:GLN:HA	1:B:36:GLN:HE21	1.71	0.54
1:N:48:LYS:HD2	1:N:52:TRP:CE2	2.43	0.54
1:A:111:ILE:CD1	1:A:120:GLU:HG3	2.36	0.54
1:H:96:GLN:H	1:H:96:GLN:CD	2.11	0.54
1:E:111:ILE:HG22	1:E:112:HIS:N	2.22	0.54
1:R:133:ARG:HH11	1:R:133:ARG:HB2	1.71	0.54
1:J:94:THR:O	1:J:98:ILE:HG12	2.08	0.54
1:O:99:ASN:HD22	1:P:96:GLN:HA	1.70	0.54
1:B:153:ARG:HH11	1:B:153:ARG:HG2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:18:ARG:NH1	1:X:18:ARG:HG3	2.22	0.54
1:M:153:ARG:NH1	1:M:153:ARG:HG2	2.22	0.54
1:U:62:VAL:HG11	1:U:118:LEU:HD11	1.90	0.54
1:B:108:PRO:HD3	1:B:124:ARG:HH22	1.73	0.54
1:F:105:LYS:O	1:F:124:ARG:NH1	2.40	0.54
1:G:48:LYS:HD2	1:G:52:TRP:CE2	2.43	0.54
1:I:22:SER:OG	1:I:25:GLU:HB2	2.08	0.54
1:S:51:HIS:O	1:S:63:HIS:HD2	1.90	0.54
1:F:153:ARG:NH1	1:F:153:ARG:HG2	2.22	0.54
1:W:43:LEU:HD11	1:W:125:TYR:CD1	2.43	0.54
1:T:60:ILE:HG23	1:T:61:ALA:N	2.23	0.54
1:P:83:ARG:NH2	1:P:143:ASP:HB2	2.23	0.54
1:I:153:ARG:HH11	1:I:153:ARG:HG2	1.73	0.54
1:B:15:LEU:HD13	1:B:88:GLY:O	2.08	0.53
1:N:96:GLN:CD	1:N:96:GLN:H	2.11	0.53
1:Q:105:LYS:O	1:Q:124:ARG:NH1	2.41	0.53
1:I:51:HIS:O	1:I:63:HIS:HD2	1.92	0.53
1:U:15:LEU:HD21	1:V:112:HIS:NE2	2.23	0.53
1:P:94:THR:O	1:P:98:ILE:HG12	2.08	0.53
1:B:48:LYS:HD2	1:B:52:TRP:CZ2	2.43	0.53
1:J:36:GLN:HA	1:J:36:GLN:NE2	2.23	0.53
1:M:83:ARG:NH2	1:M:143:ASP:HB2	2.23	0.53
1:T:153:ARG:HG3	3:T:664:HOH:O	2.07	0.53
1:V:94:THR:O	1:V:98:ILE:HG12	2.08	0.53
1:T:153:ARG:HG2	1:T:153:ARG:NH1	2.23	0.53
1:S:105:LYS:O	1:S:124:ARG:NH1	2.42	0.53
1:A:109:LEU:N	1:A:109:LEU:HD12	2.24	0.53
1:L:115:GLN:HE22	1:L:167:GLU:N	2.06	0.53
1:F:14:LEU:HD21	1:F:27:LYS:HG2	1.90	0.53
1:U:83:ARG:NH2	1:U:143:ASP:HB2	2.24	0.53
1:M:114:VAL:O	1:M:118:LEU:HD13	2.08	0.53
1:M:77:LEU:C	1:M:77:LEU:HD23	2.29	0.53
1:H:77:LEU:C	1:H:77:LEU:HD23	2.30	0.53
1:O:62:VAL:HG11	1:O:118:LEU:HD11	1.90	0.53
1:P:107:TYR:O	1:P:109:LEU:HD12	2.09	0.53
1:I:153:ARG:NH1	1:I:153:ARG:HG2	2.23	0.53
1:X:51:HIS:O	1:X:63:HIS:HD2	1.91	0.53
1:T:39:GLN:HG2	1:T:128:VAL:HG22	1.90	0.53
1:W:62:VAL:HG11	1:W:118:LEU:HD11	1.91	0.53
1:X:105:LYS:O	1:X:124:ARG:NH1	2.42	0.53
1:Q:14:LEU:HD22	1:Q:27:LYS:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:98:ILE:O	1:R:102:THR:HG22	2.09	0.53
1:T:12:THR:HG22	1:T:12:THR:O	2.09	0.53
1:G:96:GLN:H	1:G:96:GLN:CD	2.12	0.52
1:F:133:ARG:HB2	1:F:133:ARG:NH1	2.24	0.52
1:B:108:PRO:HD3	1:B:124:ARG:NH2	2.23	0.52
1:V:26:LYS:O	1:V:30:VAL:HG23	2.09	0.52
1:E:120:GLU:O	1:E:124:ARG:HG2	2.08	0.52
1:F:153:ARG:HH11	1:F:153:ARG:HG2	1.74	0.52
1:R:77:LEU:HD23	1:R:77:LEU:C	2.30	0.52
1:M:105:LYS:HE2	1:M:124:ARG:HH22	1.72	0.52
1:X:39:GLN:HG2	1:X:128:VAL:HG22	1.90	0.52
1:L:25:GLU:OE1	1:L:25:GLU:HA	2.10	0.52
1:V:77:LEU:C	1:V:77:LEU:HD23	2.30	0.52
1:F:62:VAL:HG11	1:F:118:LEU:HD11	1.91	0.52
1:M:62:VAL:HG11	1:M:118:LEU:HD11	1.91	0.52
1:B:158:PHE:O	1:B:162:ILE:HG13	2.09	0.52
1:B:39:GLN:HG2	1:B:128:VAL:HG22	1.91	0.52
1:X:120:GLU:O	1:X:124:ARG:HG2	2.09	0.52
1:R:94:THR:O	1:R:98:ILE:HG12	2.10	0.52
1:I:94:THR:O	1:I:98:ILE:HG12	2.08	0.52
1:M:105:LYS:HB3	1:M:124:ARG:NH1	2.25	0.52
1:C:36:GLN:NE2	1:C:36:GLN:HA	2.25	0.52
1:H:135:ALA:HA	1:H:138:GLU:HG2	1.91	0.52
1:F:83:ARG:NH2	1:F:143:ASP:HB2	2.24	0.52
1:X:36:GLN:NE2	1:X:36:GLN:HA	2.24	0.52
1:W:37:VAL:O	1:W:41:ILE:HG13	2.10	0.52
1:Q:55:ARG:O	1:Q:114:VAL:HG23	2.10	0.52
1:U:34:ASN:O	1:U:38:ILE:HG13	2.10	0.52
1:R:83:ARG:NH2	1:R:143:ASP:HB2	2.24	0.52
1:U:48:LYS:HE3	3:U:662:HOH:O	2.10	0.52
1:Q:153:ARG:NH1	1:Q:153:ARG:HG2	2.25	0.52
1:K:105:LYS:NZ	1:K:124:ARG:NH2	2.57	0.52
1:C:112:HIS:O	1:C:113:ASN:C	2.49	0.52
1:V:18:ARG:NH1	1:V:18:ARG:HG3	2.23	0.52
1:O:120:GLU:O	1:O:124:ARG:HG2	2.10	0.52
1:H:111:ILE:HD12	1:H:116:ASP:CB	2.38	0.52
1:C:15:LEU:HD11	1:D:112:HIS:HD2	1.74	0.52
1:N:62:VAL:HG11	1:N:118:LEU:HD11	1.92	0.52
1:B:113:ASN:OD1	1:B:115:GLN:N	2.43	0.52
1:N:133:ARG:NH1	1:N:133:ARG:HB2	2.26	0.51
1:A:18:ARG:HG3	1:A:18:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:48:LYS:HD2	1:W:52:TRP:CE2	2.45	0.51
1:I:130:ASN:OD1	1:I:133:ARG:NH2	2.43	0.51
1:P:153:ARG:HG2	1:P:153:ARG:NH1	2.25	0.51
1:R:153:ARG:NH1	1:R:153:ARG:HG2	2.25	0.51
1:W:114:VAL:O	1:W:118:LEU:HD13	2.10	0.51
1:P:120:GLU:O	1:P:124:ARG:HG2	2.10	0.51
1:M:120:GLU:O	1:M:124:ARG:HG2	2.11	0.51
1:Q:158:PHE:O	1:Q:162:ILE:HG13	2.10	0.51
1:W:19:ASN:OD1	1:W:21:VAL:HG23	2.10	0.51
1:P:105:LYS:O	1:P:124:ARG:NH1	2.43	0.51
1:Q:120:GLU:O	1:Q:124:ARG:HG2	2.11	0.51
1:G:77:LEU:C	1:G:77:LEU:HD23	2.31	0.51
1:F:48:LYS:HD2	1:F:52:TRP:CZ2	2.46	0.51
1:R:36:GLN:HE21	1:R:36:GLN:HA	1.75	0.51
1:X:36:GLN:HE21	1:X:36:GLN:HA	1.76	0.51
1:H:39:GLN:HG2	1:H:128:VAL:HG22	1.92	0.51
1:P:62:VAL:HG11	1:P:118:LEU:HD11	1.92	0.51
1:D:83:ARG:NH2	1:D:143:ASP:HB2	2.25	0.51
1:A:95:THR:HG22	1:B:99:ASN:HB2	1.91	0.51
1:Q:108:PRO:HB2	1:Q:111:ILE:HG12	1.93	0.51
1:F:133:ARG:HB2	1:F:133:ARG:HH11	1.75	0.51
1:R:109:LEU:N	1:R:109:LEU:HD12	2.26	0.51
1:H:120:GLU:O	1:H:124:ARG:HG2	2.09	0.51
1:T:62:VAL:HG11	1:T:118:LEU:HD11	1.93	0.51
1:V:120:GLU:O	1:V:124:ARG:HG2	2.11	0.51
1:Q:108:PRO:HD3	1:Q:124:ARG:NH2	2.26	0.51
1:F:120:GLU:O	1:F:124:ARG:HG2	2.10	0.51
1:G:62:VAL:HG11	1:G:118:LEU:HD11	1.93	0.51
1:X:83:ARG:NH2	1:X:143:ASP:HB2	2.25	0.51
1:N:36:GLN:NE2	1:N:36:GLN:HA	2.24	0.51
1:T:14:LEU:HD21	1:T:26:LYS:CD	2.40	0.51
1:D:108:PRO:HD3	1:D:124:ARG:HH22	1.75	0.51
1:G:105:LYS:HE3	1:G:124:ARG:NH2	2.26	0.51
1:K:108:PRO:HD3	1:K:124:ARG:NH2	2.26	0.51
1:W:94:THR:OG1	1:W:97:VAL:HG23	2.10	0.51
1:B:111:ILE:HD13	1:B:120:GLU:HG3	1.93	0.51
1:B:135:ALA:HA	1:B:138:GLU:HG2	1.92	0.51
1:S:153:ARG:HH11	1:S:153:ARG:HG2	1.76	0.51
1:D:115:GLN:HA	1:D:115:GLN:NE2	2.23	0.51
1:D:113:ASN:OD1	1:D:115:GLN:HB2	2.11	0.51
1:K:77:LEU:C	1:K:77:LEU:HD23	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:PRO:HD3	1:E:124:ARG:HH22	1.76	0.51
1:G:153:ARG:HH11	1:G:153:ARG:CG	2.24	0.51
1:N:36:GLN:HE21	1:N:36:GLN:HA	1.75	0.51
1:O:55:ARG:O	1:O:114:VAL:HG23	2.11	0.50
1:M:18:ARG:HG3	1:M:18:ARG:NH1	2.22	0.50
1:C:95:THR:OG1	1:D:42:ASP:OD1	2.29	0.50
3:F:615:HOH:O	1:L:134:LYS:HG3	2.11	0.50
1:N:120:GLU:O	1:N:124:ARG:HG2	2.12	0.50
1:G:96:GLN:HA	1:H:99:ASN:ND2	2.25	0.50
1:S:18:ARG:NH1	1:S:18:ARG:HG3	2.23	0.50
1:J:36:GLN:HA	1:J:36:GLN:HE21	1.74	0.50
1:R:153:ARG:HH11	1:R:153:ARG:HG2	1.76	0.50
1:H:82:GLU:O	1:H:86:GLN:HG3	2.11	0.50
1:I:39:GLN:HG2	1:I:128:VAL:HG22	1.93	0.50
1:G:108:PRO:HD3	1:G:124:ARG:NH2	2.27	0.50
1:Q:77:LEU:HD23	1:Q:77:LEU:C	2.32	0.50
1:P:77:LEU:C	1:P:77:LEU:HD23	2.32	0.50
1:X:130:ASN:OD1	1:X:133:ARG:NH2	2.44	0.50
1:I:120:GLU:O	1:I:124:ARG:HG2	2.11	0.50
1:D:105:LYS:O	1:D:124:ARG:NH1	2.44	0.50
1:Q:135:ALA:HA	1:Q:138:GLU:HG2	1.93	0.50
1:A:60:ILE:HG23	1:A:61:ALA:N	2.26	0.50
1:P:153:ARG:HG2	1:P:153:ARG:HH11	1.76	0.50
1:T:22:SER:OG	1:T:25:GLU:HB2	2.12	0.50
1:P:36:GLN:HA	1:P:36:GLN:HE21	1.76	0.50
1:U:102:THR:HG23	1:U:102:THR:O	2.12	0.50
1:B:60:ILE:HG23	1:B:61:ALA:N	2.27	0.50
1:W:12:THR:O	1:W:27:LYS:HE2	2.12	0.50
1:R:112:HIS:O	1:R:113:ASN:C	2.49	0.50
1:F:34:ASN:O	1:F:38:ILE:HG13	2.11	0.50
1:P:123:ASP:O	1:P:127:ILE:HD13	2.11	0.50
1:S:39:GLN:HG2	1:S:128:VAL:HG22	1.94	0.50
1:U:109:LEU:HD12	1:U:109:LEU:N	2.27	0.50
1:D:37:VAL:O	1:D:41:ILE:HG13	2.11	0.50
1:E:111:ILE:CD1	1:E:120:GLU:HG3	2.41	0.50
1:E:51:HIS:O	1:E:63:HIS:HD2	1.95	0.50
1:U:33:LEU:HD21	1:U:144:THR:CG2	2.38	0.50
1:J:130:ASN:OD1	1:J:133:ARG:NH2	2.42	0.50
1:B:26:LYS:O	1:B:30:VAL:HG23	2.12	0.50
1:B:120:GLU:O	1:B:124:ARG:HG2	2.12	0.50
1:W:60:ILE:HG23	1:W:61:ALA:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:LEU:HD23	1:I:88:GLY:O	2.11	0.50
1:K:105:LYS:O	1:K:124:ARG:NH1	2.45	0.50
1:N:26:LYS:O	1:N:30:VAL:HG23	2.11	0.50
1:M:130:ASN:OD1	1:M:133:ARG:NH2	2.43	0.50
1:S:120:GLU:O	1:S:124:ARG:HG2	2.12	0.50
1:S:22:SER:OG	1:S:25:GLU:HB2	2.11	0.50
1:A:120:GLU:O	1:A:124:ARG:HG2	2.11	0.50
1:K:98:ILE:O	1:K:102:THR:HG22	2.11	0.50
1:S:96:GLN:H	1:S:96:GLN:CD	2.15	0.50
1:O:77:LEU:C	1:O:77:LEU:HD23	2.32	0.50
1:E:158:PHE:O	1:E:162:ILE:HG13	2.12	0.50
1:T:36:GLN:NE2	1:T:36:GLN:HA	2.27	0.50
1:J:96:GLN:CD	1:J:96:GLN:H	2.15	0.49
1:T:153:ARG:HG2	1:T:153:ARG:HH11	1.77	0.49
1:F:130:ASN:OD1	1:F:133:ARG:NH2	2.44	0.49
1:F:158:PHE:O	1:F:162:ILE:HG13	2.11	0.49
1:W:83:ARG:NH2	1:W:143:ASP:HB2	2.27	0.49
1:S:113:ASN:O	1:S:116:ASP:HB2	2.12	0.49
1:O:51:HIS:O	1:O:63:HIS:HD2	1.95	0.49
1:H:36:GLN:HA	1:H:36:GLN:HE21	1.77	0.49
1:I:99:ASN:ND2	1:J:99:ASN:CB	2.73	0.49
1:D:115:GLN:HE22	1:D:166:ILE:HA	1.77	0.49
1:Q:14:LEU:HD22	1:Q:27:LYS:HE2	1.92	0.49
1:A:153:ARG:HH11	1:A:153:ARG:CG	2.24	0.49
1:W:18:ARG:HG3	1:W:18:ARG:NH1	2.26	0.49
1:I:62:VAL:HG11	1:I:118:LEU:HD11	1.94	0.49
1:M:39:GLN:HG2	1:M:128:VAL:HG22	1.94	0.49
1:N:83:ARG:NH2	1:N:143:ASP:HB2	2.27	0.49
1:G:39:GLN:HG2	1:G:128:VAL:HG22	1.94	0.49
1:O:108:PRO:HB2	1:O:111:ILE:HD11	1.93	0.49
1:E:108:PRO:HB2	1:E:111:ILE:CD1	2.42	0.49
1:O:18:ARG:HG3	1:O:18:ARG:NH1	2.26	0.49
1:C:96:GLN:H	1:C:96:GLN:CD	2.14	0.49
1:L:19:ASN:OD1	1:L:21:VAL:HG23	2.12	0.49
1:R:130:ASN:OD1	1:R:133:ARG:NH2	2.42	0.49
1:L:83:ARG:NH2	1:L:143:ASP:HB2	2.27	0.49
1:R:105:LYS:O	1:R:124:ARG:NH1	2.45	0.49
1:N:113:ASN:OD1	1:N:115:GLN:HB2	2.12	0.49
1:K:111:ILE:O	1:K:112:HIS:ND1	2.39	0.49
1:N:34:ASN:O	1:N:38:ILE:HG13	2.12	0.49
1:A:94:THR:O	1:A:98:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:ARG:NH1	1:H:18:ARG:HG3	2.28	0.49
1:Q:83:ARG:HH21	1:Q:143:ASP:HB2	1.77	0.49
1:N:51:HIS:O	1:N:63:HIS:HD2	1.95	0.49
1:K:109:LEU:CD2	1:L:92:LEU:HD22	2.39	0.49
1:F:135:ALA:HA	1:F:138:GLU:HG2	1.93	0.49
1:R:26:LYS:O	1:R:30:VAL:HG23	2.13	0.49
1:Q:96:GLN:H	1:Q:96:GLN:CD	2.14	0.49
1:T:135:ALA:HA	1:T:138:GLU:HG2	1.93	0.49
1:L:39:GLN:HG2	1:L:128:VAL:HG22	1.93	0.49
1:W:120:GLU:O	1:W:124:ARG:HG2	2.13	0.49
1:F:82:GLU:O	1:F:86:GLN:HG3	2.12	0.49
1:R:107:TYR:O	1:R:109:LEU:HD12	2.12	0.49
1:G:94:THR:O	1:G:98:ILE:HG12	2.12	0.49
1:P:48:LYS:HD2	1:P:52:TRP:CZ2	2.48	0.49
1:O:60:ILE:HG23	1:O:61:ALA:N	2.28	0.49
1:R:39:GLN:HG2	1:R:128:VAL:HG22	1.95	0.49
1:G:22:SER:C	1:G:24:SER:N	2.63	0.49
1:V:153:ARG:HG2	1:V:153:ARG:NH1	2.28	0.49
1:H:130:ASN:OD1	1:H:133:ARG:NH2	2.44	0.49
1:X:19:ASN:OD1	1:X:21:VAL:HG23	2.12	0.49
1:G:13:ASN:HB3	1:G:27:LYS:CE	2.42	0.49
1:N:77:LEU:HD23	1:N:77:LEU:C	2.33	0.49
1:O:96:GLN:H	1:O:96:GLN:CD	2.15	0.49
1:S:153:ARG:NH1	1:S:153:ARG:HG2	2.27	0.49
1:R:60:ILE:HG23	1:R:61:ALA:N	2.27	0.49
1:X:153:ARG:HG2	1:X:153:ARG:NH1	2.28	0.49
1:H:15:LEU:HD22	1:H:15:LEU:H	1.77	0.49
1:H:33:LEU:HD21	1:H:144:THR:CG2	2.39	0.49
1:L:96:GLN:H	1:L:96:GLN:CD	2.17	0.49
1:G:97:VAL:HG21	1:H:109:LEU:HD21	1.95	0.49
1:R:38:ILE:HG23	1:R:98:ILE:HA	1.94	0.49
1:O:153:ARG:CG	1:O:153:ARG:HH11	2.26	0.49
1:Q:108:PRO:HD3	1:Q:124:ARG:HH22	1.77	0.49
1:P:36:GLN:HA	1:P:36:GLN:NE2	2.28	0.49
1:G:123:ASP:O	1:G:127:ILE:HD13	2.12	0.49
1:W:39:GLN:HG2	1:W:128:VAL:HG22	1.95	0.49
1:J:39:GLN:HG2	1:J:128:VAL:HG22	1.95	0.49
1:K:83:ARG:NH2	1:K:143:ASP:HB2	2.28	0.48
1:U:96:GLN:H	1:U:96:GLN:CD	2.15	0.48
1:A:97:VAL:HG21	1:B:109:LEU:HD21	1.95	0.48
1:D:120:GLU:O	1:D:124:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:GLN:HA	1:H:36:GLN:NE2	2.28	0.48
1:T:43:LEU:HD11	1:T:125:TYR:CD1	2.47	0.48
1:T:48:LYS:HD2	1:T:52:TRP:CE2	2.48	0.48
1:I:37:VAL:O	1:I:41:ILE:HG13	2.12	0.48
1:L:15:LEU:N	1:L:15:LEU:HD22	2.28	0.48
1:E:130:ASN:OD1	1:E:133:ARG:NH2	2.44	0.48
1:C:98:ILE:O	1:C:102:THR:HG22	2.13	0.48
1:K:43:LEU:HD11	1:K:125:TYR:CD1	2.48	0.48
1:L:43:LEU:HD11	1:L:125:TYR:CD1	2.47	0.48
1:R:135:ALA:HA	1:R:138:GLU:HG2	1.95	0.48
1:A:99:ASN:N	1:B:95:THR:HG21	2.28	0.48
1:B:77:LEU:HD23	1:B:77:LEU:C	2.34	0.48
1:X:55:ARG:O	1:X:114:VAL:HG23	2.14	0.48
1:C:18:ARG:HG3	1:C:18:ARG:HH11	1.77	0.48
1:W:109:LEU:N	1:W:109:LEU:HD12	2.28	0.48
1:G:108:PRO:HD3	1:G:124:ARG:HH22	1.79	0.48
1:T:96:GLN:H	1:T:96:GLN:CD	2.15	0.48
1:B:96:GLN:CD	1:B:96:GLN:H	2.17	0.48
1:T:55:ARG:O	1:T:114:VAL:HG23	2.14	0.48
1:I:60:ILE:HG23	1:I:61:ALA:N	2.28	0.48
1:C:60:ILE:HB	1:G:165:ASN:HD21	1.78	0.48
1:P:39:GLN:HG2	1:P:128:VAL:HG22	1.95	0.48
1:V:83:ARG:NH2	1:V:143:ASP:HB2	2.27	0.48
1:G:34:ASN:O	1:G:38:ILE:HG13	2.13	0.48
1:E:62:VAL:HG11	1:E:118:LEU:HD11	1.96	0.48
1:K:105:LYS:HZ1	1:K:124:ARG:HH22	1.60	0.48
1:E:108:PRO:HB2	1:E:111:ILE:HG13	1.94	0.48
1:C:94:THR:O	1:C:98:ILE:HG12	2.13	0.48
1:W:105:LYS:O	1:W:124:ARG:NH1	2.46	0.48
1:E:48:LYS:HD2	1:E:52:TRP:CE2	2.48	0.48
1:B:107:TYR:O	1:B:109:LEU:CD1	2.61	0.48
1:C:48:LYS:HD2	1:C:52:TRP:CZ2	2.48	0.48
1:M:108:PRO:HD3	1:M:124:ARG:HH22	1.79	0.48
1:M:108:PRO:HD3	1:M:124:ARG:NH2	2.29	0.48
1:L:83:ARG:NH2	1:L:141:ASP:OD1	2.44	0.48
1:P:82:GLU:O	1:P:86:GLN:HG3	2.14	0.48
1:S:55:ARG:O	1:S:114:VAL:HG23	2.13	0.48
1:S:36:GLN:NE2	1:S:36:GLN:HA	2.28	0.48
1:G:36:GLN:HE21	1:G:36:GLN:HA	1.79	0.48
1:B:34:ASN:O	1:B:38:ILE:HG13	2.13	0.48
1:V:153:ARG:HG2	1:V:153:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HG3	1:B:18:ARG:NH1	2.27	0.48
1:F:96:GLN:H	1:F:96:GLN:CD	2.17	0.48
1:H:124:ARG:HG2	1:H:124:ARG:H	1.46	0.48
1:R:108:PRO:HD3	1:R:124:ARG:HH22	1.78	0.48
1:T:83:ARG:NH2	1:T:143:ASP:HB2	2.29	0.48
1:J:51:HIS:O	1:J:63:HIS:HD2	1.95	0.48
1:E:60:ILE:HG23	1:E:61:ALA:N	2.28	0.48
1:R:82:GLU:O	1:R:86:GLN:HG3	2.14	0.48
1:N:123:ASP:O	1:N:127:ILE:HD13	2.13	0.48
1:M:82:GLU:O	1:M:86:GLN:HG3	2.14	0.48
1:H:43:LEU:HD11	1:H:125:TYR:CD1	2.49	0.48
1:O:140:LYS:N	1:O:140:LYS:HD2	2.29	0.48
1:C:26:LYS:O	1:C:30:VAL:HG23	2.13	0.48
1:U:111:ILE:C	1:U:112:HIS:HD1	2.17	0.48
1:V:51:HIS:O	1:V:63:HIS:HD2	1.96	0.48
1:G:115:GLN:OE1	1:G:166:ILE:HA	2.13	0.48
1:I:135:ALA:HA	1:I:138:GLU:HG2	1.96	0.48
1:N:13:ASN:HD22	1:N:14:LEU:H	1.60	0.48
1:Q:112:HIS:O	1:Q:113:ASN:C	2.50	0.48
1:R:51:HIS:O	1:R:63:HIS:HD2	1.96	0.48
1:G:51:HIS:O	1:G:63:HIS:HD2	1.94	0.48
1:L:111:ILE:HD11	1:L:116:ASP:CB	2.31	0.48
1:P:96:GLN:CD	1:P:96:GLN:H	2.17	0.48
1:A:96:GLN:CD	1:A:96:GLN:H	2.17	0.48
1:D:48:LYS:HD2	1:D:52:TRP:CZ2	2.49	0.48
1:F:108:PRO:HD3	1:F:124:ARG:NH2	2.29	0.48
1:F:43:LEU:HD11	1:F:125:TYR:CD1	2.49	0.48
1:I:48:LYS:HD2	1:I:52:TRP:CE2	2.48	0.48
1:B:43:LEU:HD11	1:B:125:TYR:CD1	2.49	0.48
1:R:14:LEU:HD22	1:R:27:LYS:CE	2.44	0.47
1:D:62:VAL:HG11	1:D:118:LEU:HD11	1.95	0.47
1:K:109:LEU:HD12	1:K:109:LEU:H	1.79	0.47
1:J:83:ARG:NH2	1:J:143:ASP:HB2	2.29	0.47
1:I:19:ASN:OD1	1:I:21:VAL:HG23	2.14	0.47
1:C:60:ILE:HG23	1:C:61:ALA:N	2.29	0.47
1:U:158:PHE:O	1:U:162:ILE:HG13	2.13	0.47
1:O:39:GLN:HG2	1:O:128:VAL:HG22	1.95	0.47
1:A:62:VAL:HG11	1:A:118:LEU:HD11	1.95	0.47
1:K:140:LYS:HD2	1:K:140:LYS:N	2.29	0.47
1:T:123:ASP:O	1:T:127:ILE:HD13	2.14	0.47
1:J:10:LYS:HG3	1:J:11:ALA:N	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:572:HOH:O	1:J:48:LYS:HE3	2.14	0.47
1:U:105:LYS:HB3	1:U:124:ARG:NH1	2.29	0.47
1:M:153:ARG:HH11	1:M:153:ARG:CG	2.26	0.47
1:G:36:GLN:NE2	1:G:36:GLN:HA	2.29	0.47
1:J:60:ILE:HG23	1:J:61:ALA:N	2.29	0.47
1:O:12:THR:HG23	1:O:13:ASN:H	1.79	0.47
1:A:26:LYS:O	1:A:30:VAL:HG23	2.13	0.47
1:C:105:LYS:O	1:C:124:ARG:NH1	2.46	0.47
1:J:111:ILE:CD1	1:J:120:GLU:HG3	2.44	0.47
1:A:55:ARG:O	1:A:114:VAL:HG23	2.15	0.47
1:L:158:PHE:O	1:L:162:ILE:HG13	2.14	0.47
1:T:133:ARG:NH1	1:T:133:ARG:HB2	2.30	0.47
1:S:12:THR:HG22	1:S:12:THR:O	2.14	0.47
1:U:77:LEU:C	1:U:77:LEU:HD23	2.34	0.47
1:L:37:VAL:O	1:L:41:ILE:HG13	2.14	0.47
1:J:48:LYS:HD2	1:J:52:TRP:CZ2	2.50	0.47
1:O:118:LEU:HB3	1:O:166:ILE:HG12	1.96	0.47
1:L:118:LEU:HB3	1:L:166:ILE:HG12	1.97	0.47
1:B:118:LEU:HB3	1:B:166:ILE:HG12	1.95	0.47
1:Q:153:ARG:HH11	1:Q:153:ARG:HG2	1.78	0.47
1:N:130:ASN:OD1	1:N:133:ARG:NH2	2.47	0.47
1:I:118:LEU:HB3	1:I:166:ILE:HG12	1.97	0.47
1:O:12:THR:HG23	1:O:13:ASN:N	2.29	0.47
1:U:153:ARG:HH11	1:U:153:ARG:HG2	1.79	0.47
1:D:77:LEU:C	1:D:77:LEU:HD23	2.35	0.47
1:M:59:PHE:CD1	1:M:60:ILE:N	2.83	0.47
1:E:113:ASN:OD1	1:E:115:GLN:N	2.47	0.47
1:Q:39:GLN:HG2	1:Q:128:VAL:HG22	1.97	0.47
1:W:135:ALA:HA	1:W:138:GLU:HG2	1.96	0.47
1:S:60:ILE:HG23	1:S:61:ALA:N	2.30	0.47
1:H:115:GLN:NE2	1:H:118:LEU:HD22	2.29	0.47
1:U:99:ASN:HD22	1:V:96:GLN:HA	1.79	0.47
1:K:99:ASN:HB3	1:L:99:ASN:ND2	2.28	0.47
1:H:38:ILE:HG23	1:H:98:ILE:HA	1.97	0.47
1:Q:14:LEU:CD2	1:Q:14:LEU:N	2.78	0.47
1:E:108:PRO:HD3	1:E:124:ARG:NH2	2.29	0.47
1:V:130:ASN:OD1	1:V:133:ARG:NH2	2.46	0.47
1:R:113:ASN:OD1	1:R:115:GLN:N	2.47	0.47
1:A:130:ASN:OD1	1:A:133:ARG:NH2	2.47	0.47
1:H:108:PRO:HD3	1:H:124:ARG:NH2	2.29	0.47
1:B:112:HIS:O	1:B:113:ASN:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:133:ARG:NH1	1:I:133:ARG:HB2	2.30	0.47
1:U:153:ARG:NH1	1:U:153:ARG:HG2	2.29	0.47
1:K:60:ILE:HG23	1:K:61:ALA:N	2.30	0.47
1:T:140:LYS:N	1:T:140:LYS:HD2	2.29	0.47
1:K:153:ARG:NH1	1:K:153:ARG:HG2	2.29	0.47
1:J:34:ASN:O	1:J:38:ILE:HG13	2.15	0.47
1:O:112:HIS:O	1:O:113:ASN:C	2.51	0.47
1:D:14:LEU:HD11	1:D:27:LYS:HG3	1.96	0.47
1:K:130:ASN:OD1	1:K:133:ARG:NH2	2.44	0.47
1:B:26:LYS:HD3	1:B:87:LEU:O	2.15	0.47
1:E:51:HIS:CE1	1:E:63:HIS:NE2	2.83	0.47
1:K:62:VAL:HG11	1:K:118:LEU:HD11	1.97	0.47
1:K:36:GLN:NE2	1:K:36:GLN:HA	2.29	0.47
1:R:62:VAL:HG11	1:R:118:LEU:HD11	1.96	0.47
1:F:153:ARG:HH11	1:F:153:ARG:CG	2.26	0.47
1:S:83:ARG:NH2	1:S:143:ASP:HB2	2.30	0.47
1:O:107:TYR:HA	1:O:108:PRO:HD3	1.79	0.47
1:O:109:LEU:HD23	1:P:92:LEU:CD2	2.38	0.47
1:K:99:ASN:ND2	1:L:96:GLN:HA	2.30	0.47
1:P:19:ASN:OD1	1:P:21:VAL:HG23	2.15	0.47
1:E:99:ASN:CB	1:F:99:ASN:HD22	2.25	0.47
1:P:108:PRO:HD3	1:P:124:ARG:NH2	2.30	0.47
1:J:107:TYR:O	1:J:109:LEU:HD12	2.14	0.47
1:G:15:LEU:CD2	1:G:15:LEU:H	2.28	0.47
1:E:37:VAL:O	1:E:41:ILE:HG13	2.15	0.47
1:B:100:SER:OG	1:B:101:LYS:N	2.47	0.47
1:F:51:HIS:O	1:F:63:HIS:HD2	1.98	0.47
1:H:25:GLU:OE1	1:H:140:LYS:HB2	2.16	0.47
1:O:36:GLN:HA	1:O:36:GLN:NE2	2.29	0.47
1:A:13:ASN:HB2	1:U:22:SER:HB3	1.97	0.46
1:H:108:PRO:HD3	1:H:124:ARG:HH22	1.79	0.46
1:B:153:ARG:HH11	1:B:153:ARG:CG	2.28	0.46
1:J:153:ARG:CG	1:J:153:ARG:HH11	2.26	0.46
1:R:108:PRO:HD3	1:R:124:ARG:NH2	2.29	0.46
1:T:83:ARG:NH2	1:T:141:ASP:OD1	2.39	0.46
1:A:114:VAL:HG12	1:A:118:LEU:HD13	1.97	0.46
1:G:43:LEU:HD11	1:G:125:TYR:CD1	2.50	0.46
1:B:167:GLU:OE1	2:E:312:TRS:H31	2.14	0.46
1:A:51:HIS:O	1:A:63:HIS:HD2	1.98	0.46
1:S:140:LYS:HD2	1:S:140:LYS:N	2.30	0.46
1:E:94:THR:O	1:E:98:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:108:PRO:HB2	1:J:111:ILE:HG12	1.96	0.46
1:A:83:ARG:NH2	1:A:143:ASP:HB2	2.30	0.46
1:B:82:GLU:O	1:B:86:GLN:HG3	2.14	0.46
1:O:83:ARG:NH2	1:O:141:ASP:OD1	2.39	0.46
1:G:167:GLU:OE1	2:G:303:TRS:H21	2.15	0.46
1:C:118:LEU:HB3	1:C:166:ILE:HG12	1.97	0.46
1:E:96:GLN:CD	1:E:96:GLN:H	2.18	0.46
1:I:109:LEU:HD12	1:I:109:LEU:H	1.79	0.46
1:Q:83:ARG:NH2	1:Q:141:ASP:OD1	2.48	0.46
1:D:108:PRO:HD3	1:D:124:ARG:NH2	2.30	0.46
1:M:22:SER:OG	1:M:25:GLU:HB2	2.14	0.46
1:U:95:THR:HG22	1:V:99:ASN:HB2	1.96	0.46
1:D:38:ILE:HG23	1:D:98:ILE:HA	1.98	0.46
1:B:130:ASN:OD1	1:B:133:ARG:NH2	2.45	0.46
1:H:153:ARG:HH11	1:H:153:ARG:CG	2.27	0.46
1:K:14:LEU:HD13	1:K:15:LEU:H	1.80	0.46
1:M:35:ARG:NH2	1:M:131:ASP:OD2	2.49	0.46
1:Q:25:GLU:OE2	1:Q:140:LYS:HB3	2.15	0.46
1:O:109:LEU:N	1:O:109:LEU:HD12	2.30	0.46
1:V:38:ILE:HG23	1:V:98:ILE:HA	1.96	0.46
1:P:130:ASN:OD1	1:P:133:ARG:NH2	2.47	0.46
1:V:99:ASN:ND2	1:V:99:ASN:O	2.49	0.46
1:U:135:ALA:HA	1:U:138:GLU:HG2	1.97	0.46
1:D:135:ALA:HA	1:D:138:GLU:HG2	1.97	0.46
1:X:62:VAL:HG11	1:X:118:LEU:HD11	1.97	0.46
1:W:33:LEU:HD21	1:W:144:THR:CG2	2.42	0.46
1:D:19:ASN:OD1	1:D:21:VAL:HG23	2.16	0.46
1:K:19:ASN:OD1	1:K:21:VAL:HG23	2.16	0.46
1:L:13:ASN:O	1:L:14:LEU:HB2	2.16	0.46
1:H:60:ILE:HG23	1:H:61:ALA:N	2.30	0.46
1:L:153:ARG:NH1	1:L:153:ARG:HG2	2.30	0.46
1:K:105:LYS:HE2	1:K:124:ARG:CZ	2.45	0.46
1:G:37:VAL:O	1:G:41:ILE:HG13	2.14	0.46
1:Q:19:ASN:OD1	1:Q:21:VAL:HG23	2.16	0.46
1:I:94:THR:OG1	1:I:97:VAL:HG23	2.15	0.46
1:V:48:LYS:HD3	1:V:51:HIS:CD2	2.51	0.46
1:V:118:LEU:HB3	1:V:166:ILE:HG12	1.98	0.46
1:H:15:LEU:HD22	1:H:15:LEU:N	2.31	0.46
1:I:113:ASN:O	1:I:116:ASP:HB2	2.16	0.46
1:V:100:SER:OG	1:V:101:LYS:N	2.49	0.46
1:D:51:HIS:O	1:D:63:HIS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:113:ASN:O	1:T:116:ASP:HB2	2.15	0.46
1:R:96:GLN:CD	1:R:96:GLN:H	2.18	0.46
1:N:133:ARG:HH11	1:N:133:ARG:HB2	1.79	0.46
1:X:83:ARG:NH2	1:X:141:ASP:OD1	2.46	0.46
1:I:83:ARG:NH2	1:I:143:ASP:HB2	2.31	0.46
1:J:140:LYS:HD2	1:J:140:LYS:N	2.31	0.46
1:O:113:ASN:OD1	1:O:115:GLN:HB2	2.16	0.46
1:M:96:GLN:H	1:M:96:GLN:CD	2.19	0.46
1:B:19:ASN:OD1	1:B:21:VAL:HG23	2.16	0.46
1:T:36:GLN:HE21	1:T:36:GLN:HA	1.81	0.46
1:N:135:ALA:HA	1:N:138:GLU:HG2	1.97	0.46
1:G:135:ALA:HA	1:G:138:GLU:HG2	1.98	0.46
1:O:124:ARG:HG2	1:O:124:ARG:H	1.51	0.46
1:G:105:LYS:HE3	1:G:124:ARG:HH22	1.79	0.46
1:K:34:ASN:O	1:K:38:ILE:HG13	2.16	0.46
1:A:15:LEU:HD22	1:A:15:LEU:N	2.31	0.46
1:K:55:ARG:O	1:K:114:VAL:HG23	2.16	0.46
1:D:43:LEU:HD11	1:D:125:TYR:CD1	2.51	0.46
1:A:39:GLN:HG2	1:A:128:VAL:HG22	1.98	0.46
1:N:43:LEU:HD11	1:N:125:TYR:CD1	2.50	0.46
1:V:34:ASN:O	1:V:38:ILE:HG13	2.16	0.45
1:V:96:GLN:CD	1:V:96:GLN:H	2.19	0.45
1:H:19:ASN:OD1	1:H:21:VAL:HG23	2.16	0.45
1:E:94:THR:OG1	1:E:97:VAL:HG23	2.16	0.45
1:U:108:PRO:HB2	1:U:111:ILE:HG12	1.98	0.45
1:U:112:HIS:O	1:U:117:HIS:HD2	1.99	0.45
1:U:112:HIS:O	1:U:113:ASN:C	2.54	0.45
1:N:51:HIS:CE1	1:N:63:HIS:NE2	2.84	0.45
1:B:124:ARG:HG2	1:B:124:ARG:H	1.45	0.45
1:S:36:GLN:HE21	1:S:36:GLN:HA	1.81	0.45
1:I:83:ARG:NH2	1:I:141:ASP:OD1	2.41	0.45
1:A:43:LEU:HD11	1:A:125:TYR:CD1	2.51	0.45
1:A:35:ARG:NH2	1:A:131:ASP:OD2	2.49	0.45
1:K:83:ARG:NH2	1:K:141:ASP:OD1	2.47	0.45
1:N:94:THR:OG1	1:N:97:VAL:HG23	2.15	0.45
1:X:77:LEU:HD23	1:X:77:LEU:C	2.37	0.45
1:Q:48:LYS:HD2	1:Q:52:TRP:CZ2	2.52	0.45
1:B:83:ARG:NH2	1:B:143:ASP:HB2	2.31	0.45
1:N:35:ARG:NH2	1:N:131:ASP:OD2	2.49	0.45
1:D:153:ARG:HG2	1:D:153:ARG:NH1	2.31	0.45
1:C:19:ASN:OD1	1:C:21:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:130:ASN:OD1	1:Q:133:ARG:NH2	2.49	0.45
1:C:153:ARG:CG	1:C:153:ARG:HH11	2.29	0.45
1:M:113:ASN:OD1	1:M:115:GLN:HB2	2.16	0.45
1:N:113:ASN:OD1	1:N:115:GLN:N	2.49	0.45
1:A:83:ARG:NH2	1:A:141:ASP:OD1	2.46	0.45
1:D:153:ARG:HG3	3:D:703:HOH:O	2.15	0.45
1:W:158:PHE:O	1:W:162:ILE:HG13	2.17	0.45
1:A:123:ASP:O	1:A:127:ILE:HD13	2.16	0.45
1:U:35:ARG:NH2	1:U:131:ASP:OD2	2.50	0.45
1:W:96:GLN:H	1:W:96:GLN:CD	2.19	0.45
1:S:48:LYS:HD2	1:S:52:TRP:CZ2	2.52	0.45
1:D:111:ILE:HD12	1:D:116:ASP:HB3	1.97	0.45
1:J:135:ALA:HA	1:J:138:GLU:HG2	1.98	0.45
1:P:22:SER:C	1:P:24:SER:N	2.70	0.45
1:O:111:ILE:CD1	1:O:120:GLU:HG3	2.47	0.45
1:X:96:GLN:H	1:X:96:GLN:CD	2.19	0.45
1:L:130:ASN:OD1	1:L:133:ARG:NH2	2.49	0.45
1:C:77:LEU:HD23	1:C:77:LEU:C	2.37	0.45
1:F:108:PRO:HD3	1:F:124:ARG:HH22	1.82	0.45
1:I:133:ARG:NH1	1:I:156:ASP:OD2	2.48	0.45
1:A:124:ARG:H	1:A:124:ARG:HG2	1.50	0.45
1:T:14:LEU:HD11	1:T:26:LYS:HB3	1.94	0.45
1:J:107:TYR:O	1:J:109:LEU:CD1	2.64	0.45
1:S:22:SER:C	1:S:24:SER:H	2.18	0.45
1:D:153:ARG:HG2	1:D:153:ARG:HH11	1.81	0.45
1:G:60:ILE:HG23	1:G:61:ALA:N	2.30	0.45
1:U:51:HIS:O	1:U:63:HIS:HD2	1.99	0.45
1:Q:22:SER:C	1:Q:24:SER:N	2.70	0.45
1:D:118:LEU:HB3	1:D:166:ILE:HG12	1.98	0.45
1:F:37:VAL:O	1:F:41:ILE:HG13	2.16	0.45
1:R:118:LEU:HB3	1:R:166:ILE:HG12	1.99	0.45
1:K:107:TYR:HA	1:K:108:PRO:HD3	1.81	0.45
1:D:96:GLN:H	1:D:96:GLN:CD	2.19	0.45
1:R:94:THR:OG1	1:R:97:VAL:HG23	2.16	0.45
1:Q:108:PRO:HB2	1:Q:111:ILE:CD1	2.46	0.45
1:G:118:LEU:HB3	1:G:166:ILE:HG12	1.99	0.45
1:X:153:ARG:HG2	1:X:153:ARG:HH11	1.81	0.45
1:Q:118:LEU:HB3	1:Q:166:ILE:HG12	1.98	0.45
1:H:51:HIS:O	1:H:63:HIS:HD2	1.99	0.45
1:G:140:LYS:HD2	1:G:140:LYS:N	2.32	0.45
1:U:36:GLN:NE2	1:U:36:GLN:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97:VAL:CG2	1:L:109:LEU:HD21	2.46	0.45
1:Q:37:VAL:O	1:Q:41:ILE:HG13	2.17	0.45
1:B:62:VAL:HG11	1:B:118:LEU:HD11	1.98	0.45
1:P:111:ILE:CD1	1:P:120:GLU:HG3	2.47	0.45
1:H:105:LYS:HB3	1:H:124:ARG:NH1	2.32	0.45
1:T:107:TYR:HA	1:T:108:PRO:HD3	1.80	0.45
1:D:108:PRO:HB2	1:D:111:ILE:HG23	1.99	0.45
1:C:99:ASN:HB2	1:D:95:THR:HG22	1.99	0.45
1:I:43:LEU:HD11	1:I:125:TYR:CD1	2.52	0.45
1:F:39:GLN:HG2	1:F:128:VAL:HG22	1.99	0.45
1:W:123:ASP:O	1:W:127:ILE:HD13	2.15	0.45
1:C:115:GLN:OE1	1:C:167:GLU:HG2	2.17	0.45
1:S:99:ASN:ND2	1:T:96:GLN:HA	2.31	0.45
1:H:34:ASN:O	1:H:38:ILE:HG13	2.16	0.45
1:A:99:ASN:CB	1:B:95:THR:HG22	2.43	0.45
1:P:111:ILE:HG13	1:P:117:HIS:CE1	2.52	0.45
1:P:111:ILE:HD13	1:P:120:GLU:HG3	1.99	0.45
1:Q:43:LEU:HD11	1:Q:125:TYR:CD1	2.51	0.45
1:M:12:THR:HG23	1:M:13:ASN:N	2.31	0.45
1:C:135:ALA:HA	1:C:138:GLU:HG2	1.99	0.45
1:X:82:GLU:O	1:X:86:GLN:HG3	2.16	0.45
1:H:102:THR:HG23	1:H:102:THR:O	2.17	0.45
1:F:36:GLN:HA	1:F:36:GLN:NE2	2.32	0.45
1:G:92:LEU:HD22	1:H:109:LEU:HD23	1.98	0.45
1:I:153:ARG:CG	1:I:153:ARG:HH11	2.29	0.45
1:E:118:LEU:HB3	1:E:166:ILE:HG12	1.98	0.45
1:K:113:ASN:OD1	1:K:114:VAL:N	2.50	0.45
1:C:83:ARG:NH2	1:C:143:ASP:HB2	2.32	0.45
1:X:15:LEU:HD23	1:X:88:GLY:O	2.17	0.45
1:N:140:LYS:HD2	1:N:140:LYS:N	2.31	0.45
1:P:34:ASN:O	1:P:38:ILE:HG13	2.18	0.44
1:K:96:GLN:H	1:K:96:GLN:CD	2.19	0.44
1:X:107:TYR:HA	1:X:108:PRO:HD3	1.84	0.44
1:D:94:THR:OG1	1:D:97:VAL:HG23	2.16	0.44
1:S:130:ASN:OD1	1:S:133:ARG:NH2	2.50	0.44
1:H:37:VAL:O	1:H:41:ILE:HG13	2.17	0.44
1:S:124:ARG:H	1:S:124:ARG:HG2	1.48	0.44
1:E:70:ARG:HD2	3:E:608:HOH:O	2.16	0.44
1:W:26:LYS:HD3	1:W:87:LEU:O	2.17	0.44
1:F:105:LYS:HE2	1:F:124:ARG:NH2	2.32	0.44
1:R:43:LEU:HD11	1:R:125:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:135:ALA:HA	1:X:138:GLU:HG2	1.98	0.44
1:I:34:ASN:O	1:I:38:ILE:HG13	2.17	0.44
1:P:38:ILE:HG23	1:P:98:ILE:HA	1.98	0.44
1:T:14:LEU:HD23	1:T:15:LEU:O	2.17	0.44
1:I:96:GLN:H	1:I:96:GLN:CD	2.19	0.44
1:T:124:ARG:H	1:T:124:ARG:HG2	1.53	0.44
1:V:107:TYR:HA	1:V:108:PRO:HD3	1.76	0.44
1:H:62:VAL:HG11	1:H:118:LEU:HD11	1.99	0.44
1:L:153:ARG:HH11	1:L:153:ARG:HG2	1.83	0.44
1:N:60:ILE:HG23	1:N:61:ALA:N	2.32	0.44
1:V:135:ALA:HA	1:V:138:GLU:HG2	1.99	0.44
1:V:158:PHE:O	1:V:162:ILE:HG13	2.17	0.44
1:L:108:PRO:HD3	1:L:124:ARG:NH2	2.32	0.44
1:P:113:ASN:OD1	1:P:115:GLN:N	2.51	0.44
1:G:109:LEU:HD12	1:G:109:LEU:N	2.32	0.44
1:M:99:ASN:HB2	1:N:95:THR:HG22	1.99	0.44
1:U:124:ARG:H	1:U:124:ARG:HG2	1.48	0.44
1:P:153:ARG:HH11	1:P:153:ARG:CG	2.30	0.44
1:I:55:ARG:O	1:I:114:VAL:HG23	2.17	0.44
1:U:123:ASP:O	1:U:127:ILE:HD13	2.17	0.44
1:M:140:LYS:HD2	1:M:140:LYS:N	2.32	0.44
1:R:19:ASN:OD1	1:R:21:VAL:HG23	2.18	0.44
1:W:130:ASN:OD1	1:W:133:ARG:NH2	2.50	0.44
1:K:37:VAL:O	1:K:41:ILE:HG13	2.17	0.44
1:U:37:VAL:O	1:U:41:ILE:HG13	2.17	0.44
1:W:153:ARG:CG	1:W:153:ARG:HH11	2.29	0.44
1:K:48:LYS:HD2	1:K:52:TRP:CZ2	2.53	0.44
1:B:105:LYS:HB3	1:B:124:ARG:NH1	2.32	0.44
1:N:115:GLN:OE1	1:N:167:GLU:HG2	2.17	0.44
1:T:133:ARG:HH11	1:T:133:ARG:HB2	1.83	0.44
1:C:99:ASN:CG	1:D:99:ASN:OD1	2.56	0.44
1:H:100:SER:OG	1:H:101:LYS:N	2.49	0.44
1:V:82:GLU:O	1:V:86:GLN:HG3	2.17	0.44
1:K:135:ALA:HA	1:K:138:GLU:HG2	1.99	0.44
1:G:111:ILE:HG13	1:G:117:HIS:CE1	2.52	0.44
1:O:108:PRO:HD3	1:O:124:ARG:NH2	2.33	0.44
1:L:94:THR:OG1	1:L:97:VAL:HG23	2.18	0.44
1:W:118:LEU:HB3	1:W:166:ILE:HG12	2.00	0.44
1:H:107:TYR:HA	1:H:108:PRO:HD3	1.82	0.44
1:S:108:PRO:HD3	1:S:124:ARG:NH2	2.32	0.44
1:H:118:LEU:HB3	1:H:166:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:VAL:HG12	1:K:118:LEU:HD13	2.00	0.44
1:H:140:LYS:N	1:H:140:LYS:HD2	2.32	0.44
1:U:51:HIS:CE1	1:U:63:HIS:NE2	2.86	0.44
1:I:140:LYS:N	1:I:140:LYS:HD2	2.32	0.44
1:K:97:VAL:HG21	1:L:109:LEU:HD21	2.00	0.44
1:O:113:ASN:O	1:O:116:ASP:HB2	2.18	0.44
1:N:38:ILE:HG23	1:N:98:ILE:HA	2.00	0.44
1:O:37:VAL:O	1:O:41:ILE:HG13	2.18	0.44
1:G:15:LEU:HD23	1:G:88:GLY:O	2.17	0.44
1:B:111:ILE:CD1	1:B:120:GLU:HG3	2.48	0.44
1:T:153:ARG:CG	1:T:153:ARG:HH11	2.30	0.44
1:Q:153:ARG:CG	1:Q:153:ARG:HH11	2.30	0.44
1:D:105:LYS:HG2	1:D:106:SER:N	2.33	0.44
1:R:120:GLU:O	1:R:124:ARG:HG2	2.17	0.44
1:E:135:ALA:HA	1:E:138:GLU:HG2	2.00	0.44
1:J:118:LEU:HB3	1:J:166:ILE:HG12	1.98	0.44
1:L:111:ILE:HG13	1:L:116:ASP:HB3	2.00	0.44
1:O:99:ASN:ND2	1:P:96:GLN:CA	2.75	0.44
1:T:19:ASN:OD1	1:T:21:VAL:HG23	2.17	0.44
1:U:108:PRO:HB2	1:U:111:ILE:CD1	2.48	0.44
1:K:59:PHE:CD1	1:K:60:ILE:N	2.86	0.44
1:K:153:ARG:HH11	1:K:153:ARG:HG2	1.83	0.44
1:M:34:ASN:O	1:M:38:ILE:HG13	2.18	0.44
1:V:39:GLN:HG2	1:V:128:VAL:HG22	2.00	0.44
1:B:51:HIS:O	1:B:63:HIS:HD2	2.01	0.44
1:D:109:LEU:HD12	1:D:109:LEU:N	2.33	0.44
1:D:130:ASN:OD1	1:D:133:ARG:NH2	2.47	0.44
1:T:94:THR:OG1	1:T:97:VAL:HG23	2.18	0.44
1:U:130:ASN:OD1	1:U:133:ARG:NH2	2.46	0.44
1:P:109:LEU:N	1:P:109:LEU:HD12	2.33	0.44
1:U:108:PRO:HD3	1:U:124:ARG:HH22	1.83	0.44
1:B:105:LYS:O	1:B:124:ARG:NH1	2.50	0.44
1:I:133:ARG:HH11	1:I:133:ARG:HB2	1.83	0.44
1:T:25:GLU:HA	1:T:25:GLU:OE1	2.18	0.44
1:W:108:PRO:HD3	1:W:124:ARG:HH22	1.83	0.44
1:G:22:SER:C	1:G:24:SER:H	2.21	0.44
1:A:118:LEU:HB3	1:A:166:ILE:HG12	2.00	0.44
1:M:60:ILE:HG23	1:M:61:ALA:N	2.33	0.44
1:L:51:HIS:O	1:L:63:HIS:HD2	2.00	0.44
1:O:108:PRO:HB2	1:O:111:ILE:CD1	2.47	0.43
1:V:33:LEU:HD21	1:V:144:THR:CG2	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:133:ARG:CB	1:Q:133:ARG:NH1	2.81	0.43
1:B:94:THR:OG1	1:B:97:VAL:HG23	2.18	0.43
1:S:94:THR:OG1	1:S:97:VAL:HG23	2.18	0.43
1:I:26:LYS:HD3	1:I:87:LEU:O	2.18	0.43
1:L:77:LEU:HD23	1:L:77:LEU:C	2.38	0.43
1:V:36:GLN:HE21	1:V:36:GLN:CA	2.29	0.43
1:A:48:LYS:HD2	1:A:52:TRP:CZ2	2.52	0.43
1:O:22:SER:OG	1:O:25:GLU:CB	2.65	0.43
1:P:51:HIS:O	1:P:63:HIS:HD2	2.01	0.43
1:N:55:ARG:O	1:N:114:VAL:HG23	2.17	0.43
1:L:36:GLN:HE21	1:L:36:GLN:HA	1.83	0.43
1:C:107:TYR:O	1:C:109:LEU:CD1	2.64	0.43
1:F:19:ASN:OD1	1:F:21:VAL:HG23	2.17	0.43
1:G:26:LYS:O	1:G:30:VAL:HG23	2.18	0.43
1:M:19:ASN:OD1	1:M:21:VAL:HG23	2.18	0.43
1:U:48:LYS:HD2	1:U:52:TRP:CZ2	2.52	0.43
1:B:108:PRO:C	1:B:110:ASP:H	2.20	0.43
1:K:36:GLN:HE21	1:K:36:GLN:HA	1.82	0.43
1:C:51:HIS:O	1:C:63:HIS:HD2	2.01	0.43
1:S:135:ALA:HA	1:S:138:GLU:HG2	1.99	0.43
1:E:140:LYS:N	1:E:140:LYS:HD2	2.33	0.43
1:Q:33:LEU:HD21	1:Q:144:THR:CG2	2.43	0.43
1:V:35:ARG:NH2	1:V:131:ASP:OD2	2.50	0.43
1:C:130:ASN:OD1	1:C:133:ARG:NH2	2.49	0.43
1:T:77:LEU:C	1:T:77:LEU:HD23	2.39	0.43
1:M:48:LYS:HD2	1:M:52:TRP:CZ2	2.54	0.43
1:V:108:PRO:HD3	1:V:124:ARG:NH2	2.34	0.43
1:N:108:PRO:HD3	1:N:124:ARG:HH22	1.83	0.43
1:U:36:GLN:HE21	1:U:36:GLN:HA	1.83	0.43
1:O:135:ALA:HA	1:O:138:GLU:HG2	2.00	0.43
1:P:135:ALA:HA	1:P:138:GLU:HG2	1.99	0.43
1:D:35:ARG:NH2	1:D:131:ASP:OD2	2.50	0.43
1:O:43:LEU:HD11	1:O:125:TYR:CD1	2.54	0.43
1:U:13:ASN:H	1:U:27:LYS:CE	2.31	0.43
1:O:14:LEU:HD21	1:O:27:LYS:HG2	2.01	0.43
1:O:130:ASN:OD1	1:O:133:ARG:NH2	2.50	0.43
1:I:51:HIS:CE1	1:I:63:HIS:NE2	2.86	0.43
1:R:153:ARG:HG3	3:R:691:HOH:O	2.19	0.43
1:N:107:TYR:HA	1:N:108:PRO:HD3	1.77	0.43
1:N:124:ARG:H	1:N:124:ARG:HG2	1.60	0.43
1:K:158:PHE:O	1:K:162:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:THR:O	1:E:102:THR:HG23	2.18	0.43
1:J:123:ASP:O	1:J:127:ILE:HD13	2.19	0.43
1:X:112:HIS:O	1:X:113:ASN:C	2.55	0.43
1:L:135:ALA:HA	1:L:138:GLU:HG2	2.00	0.43
1:A:135:ALA:HA	1:A:138:GLU:HG2	1.99	0.43
1:P:94:THR:OG1	1:P:97:VAL:HG23	2.18	0.43
1:A:77:LEU:HD23	1:A:77:LEU:C	2.39	0.43
1:W:36:GLN:HE21	1:W:36:GLN:CA	2.28	0.43
1:Q:124:ARG:H	1:Q:124:ARG:HG2	1.49	0.43
1:B:113:ASN:OD1	1:B:115:GLN:HB2	2.19	0.43
1:K:51:HIS:O	1:K:63:HIS:HD2	2.01	0.43
1:K:33:LEU:HD13	1:K:83:ARG:HB3	2.00	0.43
1:Q:34:ASN:O	1:Q:38:ILE:HG13	2.18	0.43
1:C:111:ILE:HD13	1:C:120:GLU:HG3	2.00	0.43
1:P:83:ARG:HH21	1:P:143:ASP:HB2	1.83	0.43
1:R:12:THR:HG22	1:R:13:ASN:N	2.33	0.43
1:F:54:MET:HA	1:F:112:HIS:O	2.19	0.43
1:F:140:LYS:N	1:F:140:LYS:HD2	2.33	0.43
1:V:140:LYS:N	1:V:140:LYS:HD2	2.34	0.43
1:O:15:LEU:HD23	1:P:55:ARG:NE	2.25	0.43
1:K:38:ILE:HG23	1:K:98:ILE:HA	2.01	0.43
1:X:109:LEU:HD12	1:X:109:LEU:N	2.33	0.43
1:D:38:ILE:HG23	1:D:98:ILE:HD13	2.01	0.43
1:F:25:GLU:HA	1:F:25:GLU:OE1	2.19	0.43
1:S:118:LEU:HB3	1:S:166:ILE:HG12	2.00	0.43
1:V:108:PRO:HD3	1:V:124:ARG:HH22	1.83	0.43
1:P:114:VAL:O	1:P:118:LEU:HD13	2.18	0.43
1:W:124:ARG:H	1:W:124:ARG:HG2	1.45	0.43
1:T:130:ASN:OD1	1:T:133:ARG:NH2	2.50	0.43
1:K:118:LEU:HB3	1:K:166:ILE:HG12	2.00	0.43
1:O:83:ARG:NH2	1:O:143:ASP:HB2	2.34	0.43
1:D:99:ASN:O	1:D:102:THR:HG22	2.18	0.43
1:F:36:GLN:HA	1:F:36:GLN:HE21	1.83	0.43
1:O:82:GLU:O	1:O:86:GLN:HG3	2.19	0.43
1:T:160:TRP:CZ3	1:T:161:PHE:HE1	2.37	0.43
2:P:318:TRS:H21	1:U:167:GLU:OE1	2.19	0.43
1:C:34:ASN:O	1:C:38:ILE:HG13	2.18	0.43
1:W:140:LYS:N	1:W:140:LYS:HD2	2.34	0.43
1:J:26:LYS:O	1:J:30:VAL:HG23	2.18	0.43
1:F:38:ILE:HG23	1:F:98:ILE:HA	1.99	0.43
1:O:26:LYS:HD3	1:O:87:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:LYS:HD2	1:H:52:TRP:CZ2	2.53	0.43
1:E:43:LEU:HD11	1:E:125:TYR:CE1	2.54	0.43
1:J:43:LEU:HD11	1:J:125:TYR:CD1	2.54	0.43
1:V:113:ASN:OD1	1:V:115:GLN:N	2.51	0.43
1:E:123:ASP:O	1:E:127:ILE:HD13	2.19	0.43
1:J:158:PHE:O	1:J:162:ILE:HG13	2.18	0.43
1:O:35:ARG:NH2	1:O:131:ASP:OD2	2.51	0.43
1:M:43:LEU:HD11	1:M:125:TYR:CD1	2.54	0.43
1:K:124:ARG:H	1:K:124:ARG:HG2	1.53	0.43
1:J:124:ARG:HG2	1:J:124:ARG:H	1.46	0.43
1:N:39:GLN:CG	1:N:128:VAL:HG22	2.49	0.43
1:N:108:PRO:HD3	1:N:124:ARG:NH2	2.34	0.43
1:D:51:HIS:CE1	1:D:63:HIS:NE2	2.87	0.43
1:T:35:ARG:NH2	1:T:131:ASP:OD2	2.52	0.43
1:C:140:LYS:HD2	1:C:140:LYS:N	2.33	0.43
1:Q:38:ILE:HG23	1:Q:98:ILE:HA	1.99	0.42
1:D:34:ASN:O	1:D:38:ILE:HG13	2.19	0.42
1:Q:109:LEU:CD2	1:R:92:LEU:HD22	2.49	0.42
1:I:108:PRO:HD3	1:I:124:ARG:NH2	2.34	0.42
1:U:118:LEU:HB3	1:U:166:ILE:HG12	2.00	0.42
1:O:108:PRO:HD3	1:O:124:ARG:HH22	1.84	0.42
1:W:133:ARG:CB	1:W:133:ARG:NH1	2.79	0.42
1:W:26:LYS:O	1:W:30:VAL:HG23	2.19	0.42
1:P:37:VAL:O	1:P:41:ILE:HG13	2.18	0.42
1:R:83:ARG:NH2	1:R:141:ASP:OD1	2.43	0.42
1:W:108:PRO:HD3	1:W:124:ARG:NH2	2.34	0.42
1:B:123:ASP:O	1:B:127:ILE:HD13	2.19	0.42
1:R:35:ARG:NH2	1:R:131:ASP:OD2	2.52	0.42
1:N:76:HIS:O	1:N:80:MET:HG3	2.19	0.42
1:P:33:LEU:HD21	1:P:144:THR:CG2	2.43	0.42
1:G:107:TYR:HA	1:G:108:PRO:HD3	1.80	0.42
1:P:109:LEU:H	1:P:109:LEU:HD12	1.83	0.42
1:U:111:ILE:CD1	1:U:120:GLU:HG3	2.49	0.42
1:U:108:PRO:HD3	1:U:124:ARG:NH2	2.34	0.42
1:N:107:TYR:O	1:N:109:LEU:HD13	2.19	0.42
1:C:18:ARG:NH1	1:C:18:ARG:HG3	2.35	0.42
1:O:36:GLN:HA	1:O:36:GLN:HE21	1.83	0.42
1:L:36:GLN:NE2	1:L:36:GLN:HA	2.33	0.42
1:X:113:ASN:OD1	1:X:115:GLN:N	2.53	0.42
1:D:39:GLN:HG2	1:D:128:VAL:HG22	2.00	0.42
1:D:158:PHE:O	1:D:162:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:55:ARG:HD2	1:O:112:HIS:HD2	1.83	0.42
1:T:34:ASN:O	1:T:38:ILE:HG13	2.19	0.42
1:S:77:LEU:HD23	1:S:77:LEU:C	2.39	0.42
1:A:14:LEU:HD21	1:A:27:LYS:HG3	2.01	0.42
1:I:109:LEU:HD12	1:I:109:LEU:N	2.34	0.42
1:T:158:PHE:O	1:T:162:ILE:HG13	2.19	0.42
1:X:60:ILE:HG23	1:X:61:ALA:N	2.34	0.42
1:C:158:PHE:O	1:C:162:ILE:HG13	2.19	0.42
1:U:12:THR:HB	1:U:27:LYS:CE	2.48	0.42
1:C:108:PRO:HD3	1:C:124:ARG:NH2	2.34	0.42
1:X:12:THR:OG1	1:X:27:LYS:HD3	2.19	0.42
1:E:19:ASN:OD1	1:E:21:VAL:HG23	2.19	0.42
1:C:15:LEU:HD23	1:C:88:GLY:O	2.19	0.42
1:G:15:LEU:HD22	1:G:15:LEU:H	1.83	0.42
1:O:51:HIS:CE1	1:O:63:HIS:NE2	2.88	0.42
1:L:34:ASN:O	1:L:38:ILE:HG13	2.19	0.42
1:K:99:ASN:HD22	1:L:96:GLN:HA	1.84	0.42
1:A:19:ASN:OD1	1:A:21:VAL:HG23	2.19	0.42
1:N:19:ASN:OD1	1:N:21:VAL:HG23	2.19	0.42
1:A:94:THR:OG1	1:A:97:VAL:HG23	2.19	0.42
1:F:94:THR:OG1	1:F:97:VAL:HG23	2.19	0.42
1:X:51:HIS:CE1	1:X:63:HIS:NE2	2.88	0.42
1:K:14:LEU:HD13	1:K:15:LEU:N	2.34	0.42
1:C:43:LEU:HD11	1:C:125:TYR:CD1	2.54	0.42
1:F:113:ASN:OD1	1:F:115:GLN:N	2.49	0.42
1:V:94:THR:OG1	1:V:97:VAL:HG23	2.20	0.42
1:K:111:ILE:CD1	1:K:120:GLU:HG3	2.48	0.42
1:E:107:TYR:HA	1:E:108:PRO:HD3	1.79	0.42
1:A:36:GLN:NE2	1:A:36:GLN:HA	2.34	0.42
1:V:19:ASN:OD1	1:V:21:VAL:HG23	2.20	0.42
1:S:153:ARG:CG	1:S:153:ARG:HH11	2.33	0.42
1:C:59:PHE:CD1	1:C:60:ILE:N	2.87	0.42
1:U:153:ARG:HG3	3:U:524:HOH:O	2.19	0.42
1:U:107:TYR:O	1:U:109:LEU:CD1	2.56	0.42
1:A:108:PRO:HD3	1:A:124:ARG:HH22	1.84	0.42
1:E:14:LEU:HD23	1:E:14:LEU:N	2.28	0.42
1:S:62:VAL:HG11	1:S:118:LEU:HD11	2.02	0.42
1:H:83:ARG:HH21	1:H:143:ASP:HB2	1.83	0.42
1:P:76:HIS:O	1:P:80:MET:HG3	2.19	0.42
1:Q:123:ASP:O	1:Q:127:ILE:HD13	2.20	0.42
1:B:140:LYS:HD2	1:B:140:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:115:GLN:HA	1:P:115:GLN:OE1	2.20	0.42
1:S:26:LYS:HD3	1:S:87:LEU:O	2.20	0.42
1:V:108:PRO:HB2	1:V:111:ILE:HG12	2.01	0.42
1:P:57:ALA:O	1:P:114:VAL:HG21	2.20	0.42
1:J:35:ARG:NH2	1:J:131:ASP:OD2	2.53	0.42
1:R:14:LEU:HD22	1:R:27:LYS:HE2	2.00	0.41
1:J:33:LEU:HD13	1:J:83:ARG:HB3	2.02	0.41
1:D:36:GLN:CA	1:D:36:GLN:HE21	2.22	0.41
1:J:108:PRO:HD3	1:J:124:ARG:NH2	2.35	0.41
1:L:62:VAL:HG11	1:L:118:LEU:HD11	2.02	0.41
1:P:66:LEU:HA	1:P:66:LEU:HD12	1.94	0.41
1:U:60:ILE:HG23	1:U:61:ALA:N	2.35	0.41
1:T:14:LEU:HD11	1:T:26:LYS:CD	2.50	0.41
1:A:29:THR:HG23	1:A:144:THR:HG21	2.02	0.41
1:R:54:MET:HB2	1:R:114:VAL:HG22	2.02	0.41
1:L:97:VAL:HG13	1:L:101:LYS:HD2	2.01	0.41
1:L:38:ILE:HG23	1:L:98:ILE:HA	2.02	0.41
1:X:124:ARG:HG2	1:X:124:ARG:H	1.46	0.41
1:L:55:ARG:O	1:L:114:VAL:HG23	2.19	0.41
1:R:153:ARG:CG	1:R:153:ARG:HH11	2.32	0.41
1:S:22:SER:C	1:S:24:SER:N	2.74	0.41
1:N:12:THR:OG1	1:N:13:ASN:N	2.53	0.41
1:J:38:ILE:HG23	1:J:98:ILE:HA	2.01	0.41
1:P:140:LYS:HD2	1:P:140:LYS:N	2.34	0.41
1:Q:14:LEU:HD22	1:Q:27:LYS:HE3	2.01	0.41
1:P:108:PRO:HB2	1:P:111:ILE:CD1	2.50	0.41
1:S:109:LEU:HD23	1:T:92:LEU:HD22	2.02	0.41
1:Q:59:PHE:CD1	1:Q:60:ILE:N	2.89	0.41
1:E:48:LYS:HE3	3:F:728:HOH:O	2.19	0.41
1:X:35:ARG:NH2	1:X:131:ASP:OD2	2.53	0.41
1:U:39:GLN:HG2	1:U:128:VAL:HG22	2.02	0.41
1:X:26:LYS:HD3	1:X:87:LEU:O	2.21	0.41
1:A:14:LEU:H	1:A:14:LEU:HG	1.49	0.41
1:C:39:GLN:HG2	1:C:128:VAL:HG22	2.03	0.41
1:Q:95:THR:HG21	1:R:99:ASN:N	2.35	0.41
1:S:115:GLN:NE2	1:S:166:ILE:HA	2.33	0.41
1:C:94:THR:OG1	1:C:97:VAL:HG23	2.21	0.41
1:X:48:LYS:HD2	1:X:52:TRP:CZ2	2.55	0.41
1:V:51:HIS:CE1	1:V:63:HIS:CE1	3.09	0.41
1:G:15:LEU:CD2	1:G:15:LEU:N	2.82	0.41
1:L:114:VAL:O	1:L:117:HIS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:95:THR:OG1	1:T:42:ASP:OD1	2.32	0.41
1:A:114:VAL:O	1:A:118:LEU:HD13	2.21	0.41
1:K:42:ASP:OD1	1:L:95:THR:OG1	2.31	0.41
1:S:34:ASN:O	1:S:38:ILE:HG13	2.20	0.41
1:I:158:PHE:O	1:I:162:ILE:HG13	2.20	0.41
1:A:13:ASN:HA	1:A:27:LYS:HE2	2.02	0.41
1:M:94:THR:OG1	1:M:97:VAL:HG23	2.21	0.41
1:U:19:ASN:OD1	1:U:21:VAL:HG23	2.20	0.41
1:M:124:ARG:HG2	1:M:124:ARG:H	1.45	0.41
1:J:107:TYR:HA	1:J:108:PRO:HD3	1.80	0.41
1:R:48:LYS:HD2	1:R:52:TRP:CZ2	2.56	0.41
1:S:108:PRO:HD3	1:S:124:ARG:HH22	1.85	0.41
1:K:51:HIS:CE1	1:K:63:HIS:NE2	2.88	0.41
1:R:100:SER:OG	1:R:101:LYS:N	2.52	0.41
1:B:35:ARG:NH2	1:B:131:ASP:OD2	2.54	0.41
1:J:110:ASP:OD2	1:J:110:ASP:N	2.52	0.41
1:Q:66:LEU:HD12	1:Q:66:LEU:HA	1.90	0.41
1:A:108:PRO:HD3	1:A:124:ARG:NH2	2.36	0.41
1:C:29:THR:HG23	1:C:144:THR:HG21	2.03	0.41
1:K:105:LYS:CE	1:K:124:ARG:HH22	2.34	0.41
1:X:108:PRO:HD3	1:X:124:ARG:NH2	2.35	0.41
1:O:12:THR:OG1	1:O:13:ASN:N	2.53	0.41
1:X:59:PHE:CD1	1:X:60:ILE:N	2.89	0.41
1:U:140:LYS:HD2	1:U:140:LYS:N	2.36	0.41
1:L:108:PRO:HB2	1:L:111:ILE:HG21	2.02	0.41
1:C:109:LEU:CD1	1:C:109:LEU:N	2.83	0.41
1:G:33:LEU:HD13	1:G:83:ARG:HB3	2.02	0.41
1:S:99:ASN:N	1:T:95:THR:HG21	2.36	0.41
1:M:29:THR:HG23	1:M:144:THR:HG21	2.03	0.41
1:G:94:THR:OG1	1:G:97:VAL:HG23	2.21	0.41
1:B:38:ILE:HG23	1:B:98:ILE:HA	2.03	0.41
1:J:19:ASN:OD1	1:J:21:VAL:HG23	2.20	0.41
1:W:74:ILE:HA	1:W:77:LEU:HD13	2.02	0.41
1:W:77:LEU:C	1:W:77:LEU:HD23	2.42	0.41
1:T:108:PRO:HD3	1:T:124:ARG:HH22	1.86	0.41
1:N:118:LEU:HB3	1:N:166:ILE:HG12	2.01	0.41
1:N:36:GLN:HE21	1:N:36:GLN:CA	2.32	0.41
1:W:111:ILE:HD13	1:W:120:GLU:HG3	2.03	0.41
1:J:62:VAL:HG11	1:J:118:LEU:HD11	2.03	0.41
1:C:43:LEU:HD22	1:C:128:VAL:HG21	2.03	0.41
1:I:123:ASP:O	1:I:127:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:PHE:O	1:H:162:ILE:HG13	2.21	0.41
1:X:123:ASP:O	1:X:127:ILE:HD13	2.21	0.41
1:W:66:LEU:HA	1:W:66:LEU:HD12	1.92	0.41
1:O:158:PHE:O	1:O:162:ILE:HG13	2.21	0.41
1:E:39:GLN:HG2	1:E:128:VAL:HG22	2.03	0.41
1:A:113:ASN:O	1:A:116:ASP:HB2	2.20	0.41
1:H:26:LYS:O	1:H:30:VAL:HG23	2.20	0.41
1:A:95:THR:HG21	1:B:99:ASN:N	2.35	0.41
1:T:120:GLU:O	1:T:124:ARG:HG2	2.21	0.41
1:L:39:GLN:CG	1:L:128:VAL:HG22	2.51	0.41
1:L:158:PHE:N	1:L:158:PHE:CD2	2.90	0.41
1:D:158:PHE:N	1:D:158:PHE:CD2	2.86	0.41
1:L:140:LYS:N	1:L:140:LYS:HD2	2.35	0.41
1:R:14:LEU:CD2	1:R:27:LYS:HE3	2.51	0.40
1:T:38:ILE:HG23	1:T:98:ILE:HA	2.03	0.40
1:N:26:LYS:HD3	1:N:87:LEU:O	2.21	0.40
1:O:48:LYS:HD2	1:O:52:TRP:CZ2	2.56	0.40
1:L:26:LYS:HD3	1:L:87:LEU:O	2.21	0.40
1:Q:60:ILE:CG2	1:Q:61:ALA:N	2.85	0.40
1:N:48:LYS:HD3	1:N:51:HIS:CD2	2.56	0.40
1:M:118:LEU:HB3	1:M:166:ILE:HG12	2.03	0.40
1:N:133:ARG:NH1	1:N:156:ASP:OD2	2.54	0.40
1:B:60:ILE:HB	1:E:165:ASN:HD21	1.86	0.40
1:A:158:PHE:O	1:A:162:ILE:HG13	2.21	0.40
1:D:66:LEU:HA	1:D:66:LEU:HD12	1.93	0.40
1:K:108:PRO:HD3	1:K:124:ARG:HH22	1.84	0.40
1:F:13:ASN:O	1:F:14:LEU:O	2.40	0.40
1:H:38:ILE:HG23	1:H:98:ILE:HD13	2.03	0.40
1:E:111:ILE:O	1:E:112:HIS:ND1	2.54	0.40
1:W:108:PRO:HB2	1:W:111:ILE:HG12	2.04	0.40
1:O:13:ASN:HA	1:O:13:ASN:HD22	1.67	0.40
1:M:60:ILE:HB	1:T:165:ASN:HD21	1.85	0.40
1:C:62:VAL:HG11	1:C:118:LEU:HD11	2.03	0.40
1:S:158:PHE:O	1:S:162:ILE:HG13	2.21	0.40
1:Q:167:GLU:OE1	2:Q:324:TRS:H21	2.20	0.40
1:G:101:LYS:O	1:G:103:PRO:HD3	2.21	0.40
1:D:140:LYS:HD2	1:D:140:LYS:N	2.36	0.40
1:O:108:PRO:HB2	1:O:111:ILE:HG12	2.03	0.40
1:T:14:LEU:HD11	1:T:26:LYS:HD2	2.04	0.40
1:G:83:ARG:HH21	1:G:143:ASP:HB2	1.85	0.40
1:M:33:LEU:HD13	1:M:83:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:94:THR:OG1	1:U:97:VAL:HG23	2.21	0.40
1:E:109:LEU:N	1:E:109:LEU:CD1	2.81	0.40
1:T:108:PRO:HD3	1:T:124:ARG:NH2	2.35	0.40
1:T:114:VAL:O	1:T:118:LEU:HD13	2.22	0.40
1:K:153:ARG:HH11	1:K:153:ARG:CG	2.35	0.40
1:L:153:ARG:HH11	1:L:153:ARG:CG	2.34	0.40
1:N:22:SER:OG	1:N:25:GLU:HB2	2.22	0.40
1:L:123:ASP:O	1:L:127:ILE:HD13	2.21	0.40
1:R:14:LEU:HD22	1:R:27:LYS:HE3	2.04	0.40
1:R:114:VAL:O	1:R:118:LEU:HD13	2.20	0.40
1:J:10:LYS:CG	1:J:11:ALA:N	2.85	0.40
1:X:108:PRO:HD3	1:X:124:ARG:HH22	1.85	0.40
1:V:48:LYS:HD2	1:V:52:TRP:CZ2	2.57	0.40
1:V:83:ARG:HH21	1:V:143:ASP:HB2	1.86	0.40
1:P:60:ILE:HG23	1:P:61:ALA:N	2.36	0.40
1:W:51:HIS:O	1:W:63:HIS:HD2	2.04	0.40
1:O:66:LEU:HA	1:O:66:LEU:HD12	1.94	0.40
1:X:140:LYS:HD2	1:X:140:LYS:N	2.36	0.40
1:U:12:THR:HB	1:U:27:LYS:HE3	2.03	0.40
1:P:26:LYS:O	1:P:30:VAL:HG23	2.22	0.40
1:P:118:LEU:HB3	1:P:166:ILE:HG12	2.03	0.40
1:X:153:ARG:CG	1:X:153:ARG:HH11	2.35	0.40
1:A:112:HIS:O	1:A:113:ASN:C	2.59	0.40
1:A:157:LYS:HD2	3:I:525:HOH:O	2.21	0.40
1:R:123:ASP:O	1:R:127:ILE:HD13	2.21	0.40
1:M:135:ALA:HA	1:M:138:GLU:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/167 (92%)	142 (93%)	11 (7%)	0	100	100
1	B	153/167 (92%)	141 (92%)	10 (6%)	2 (1%)	15	30
1	C	152/167 (91%)	140 (92%)	12 (8%)	0	100	100
1	D	152/167 (91%)	138 (91%)	13 (9%)	1 (1%)	26	51
1	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
1	F	153/167 (92%)	149 (97%)	3 (2%)	1 (1%)	26	51
1	G	153/167 (92%)	142 (93%)	11 (7%)	0	100	100
1	H	152/167 (91%)	140 (92%)	11 (7%)	1 (1%)	26	51
1	I	152/167 (91%)	144 (95%)	8 (5%)	0	100	100
1	J	156/167 (93%)	148 (95%)	7 (4%)	1 (1%)	30	56
1	K	152/167 (91%)	144 (95%)	8 (5%)	0	100	100
1	L	153/167 (92%)	142 (93%)	8 (5%)	3 (2%)	9	18
1	M	154/167 (92%)	145 (94%)	8 (5%)	1 (1%)	30	56
1	N	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
1	O	154/167 (92%)	146 (95%)	8 (5%)	0	100	100
1	P	152/167 (91%)	145 (95%)	7 (5%)	0	100	100
1	Q	152/167 (91%)	140 (92%)	11 (7%)	1 (1%)	26	51
1	R	154/167 (92%)	148 (96%)	6 (4%)	0	100	100
1	S	154/167 (92%)	144 (94%)	10 (6%)	0	100	100
1	T	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
1	U	155/167 (93%)	142 (92%)	12 (8%)	1 (1%)	30	56
1	V	153/167 (92%)	145 (95%)	8 (5%)	0	100	100
1	W	154/167 (92%)	144 (94%)	9 (6%)	1 (1%)	30	56
1	X	154/167 (92%)	144 (94%)	10 (6%)	0	100	100
All	All	3679/4008 (92%)	3460 (94%)	206 (6%)	13 (0%)	39	65

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	14	LEU
1	D	101	LYS
1	L	114	VAL
1	H	101	LYS
1	J	14	LEU
1	L	14	LEU

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Mol	Chain	Res	Type
1	Q	113	ASN
1	B	101	LYS
1	M	100	SER
1	U	113	ASN
1	L	115	GLN
1	W	20	ASP
1	B	108	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	132/142 (93%)	122 (92%)	10 (8%)	16	32
1	B	132/142 (93%)	123 (93%)	9 (7%)	20	39
1	C	131/142 (92%)	122 (93%)	9 (7%)	19	38
1	D	131/142 (92%)	123 (94%)	8 (6%)	23	46
1	E	133/142 (94%)	125 (94%)	8 (6%)	24	47
1	F	132/142 (93%)	125 (95%)	7 (5%)	28	53
1	G	132/142 (93%)	125 (95%)	7 (5%)	28	53
1	H	131/142 (92%)	123 (94%)	8 (6%)	23	46
1	I	131/142 (92%)	124 (95%)	7 (5%)	28	53
1	J	134/142 (94%)	126 (94%)	8 (6%)	24	47
1	K	131/142 (92%)	121 (92%)	10 (8%)	16	32
1	L	132/142 (93%)	122 (92%)	10 (8%)	16	32
1	M	133/142 (94%)	126 (95%)	7 (5%)	28	53
1	N	133/142 (94%)	125 (94%)	8 (6%)	24	47
1	O	133/142 (94%)	125 (94%)	8 (6%)	24	47
1	P	131/142 (92%)	123 (94%)	8 (6%)	23	46
1	Q	131/142 (92%)	122 (93%)	9 (7%)	19	38
1	R	133/142 (94%)	126 (95%)	7 (5%)	28	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	133/142 (94%)	126 (95%)	7 (5%)	28	53
1	T	133/142 (94%)	126 (95%)	7 (5%)	28	53
1	U	133/142 (94%)	124 (93%)	9 (7%)	20	39
1	V	132/142 (93%)	124 (94%)	8 (6%)	23	46
1	W	133/142 (94%)	126 (95%)	7 (5%)	28	53
1	X	133/142 (94%)	126 (95%)	7 (5%)	28	53
All	All	3173/3408 (93%)	2980 (94%)	193 (6%)	23	46

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	23	ASP
1	A	66	LEU
1	A	67	ASP
1	A	73	LEU
1	A	96	GLN
1	A	99	ASN
1	A	110	ASP
1	A	116	ASP
1	A	153	ARG
1	B	14	LEU
1	B	66	LEU
1	B	67	ASP
1	B	73	LEU
1	B	77	LEU
1	B	96	GLN
1	B	102	THR
1	B	112	HIS
1	B	153	ARG
1	C	23	ASP
1	C	66	LEU
1	C	67	ASP
1	C	73	LEU
1	C	77	LEU
1	C	96	GLN
1	C	102	THR
1	C	110	ASP
1	C	153	ARG
1	D	23	ASP

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Mol	Chain	Res	Type
1	D	66	LEU
1	D	67	ASP
1	D	73	LEU
1	D	77	LEU
1	D	96	GLN
1	D	115	GLN
1	D	153	ARG
1	E	14	LEU
1	E	66	LEU
1	E	67	ASP
1	E	73	LEU
1	E	77	LEU
1	E	96	GLN
1	E	99	ASN
1	E	153	ARG
1	F	66	LEU
1	F	67	ASP
1	F	73	LEU
1	F	77	LEU
1	F	96	GLN
1	F	109	LEU
1	F	153	ARG
1	G	14	LEU
1	G	66	LEU
1	G	67	ASP
1	G	73	LEU
1	G	77	LEU
1	G	96	GLN
1	G	153	ARG
1	H	23	ASP
1	H	66	LEU
1	H	67	ASP
1	H	73	LEU
1	H	77	LEU
1	H	96	GLN
1	H	112	HIS
1	H	153	ARG
1	I	66	LEU
1	I	67	ASP
1	I	73	LEU
1	I	77	LEU
1	I	96	GLN

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Mol	Chain	Res	Type
1	I	110	ASP
1	I	153	ARG
1	J	23	ASP
1	J	66	LEU
1	J	67	ASP
1	J	73	LEU
1	J	77	LEU
1	J	96	GLN
1	J	102	THR
1	J	153	ARG
1	K	14	LEU
1	K	23	ASP
1	K	66	LEU
1	K	67	ASP
1	K	73	LEU
1	K	77	LEU
1	K	96	GLN
1	K	111	ILE
1	K	112	HIS
1	K	153	ARG
1	L	14	LEU
1	L	66	LEU
1	L	67	ASP
1	L	73	LEU
1	L	77	LEU
1	L	96	GLN
1	L	110	ASP
1	L	111	ILE
1	L	112	HIS
1	L	153	ARG
1	M	23	ASP
1	M	66	LEU
1	M	67	ASP
1	M	73	LEU
1	M	77	LEU
1	M	96	GLN
1	M	153	ARG
1	N	13	ASN
1	N	66	LEU
1	N	67	ASP
1	N	73	LEU
1	N	77	LEU

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Mol	Chain	Res	Type
1	N	96	GLN
1	N	109	LEU
1	N	153	ARG
1	O	15	LEU
1	O	66	LEU
1	O	67	ASP
1	O	73	LEU
1	O	77	LEU
1	O	96	GLN
1	O	111	ILE
1	O	153	ARG
1	P	15	LEU
1	P	66	LEU
1	P	67	ASP
1	P	73	LEU
1	P	77	LEU
1	P	96	GLN
1	P	99	ASN
1	P	153	ARG
1	Q	14	LEU
1	Q	15	LEU
1	Q	23	ASP
1	Q	66	LEU
1	Q	67	ASP
1	Q	73	LEU
1	Q	77	LEU
1	Q	96	GLN
1	Q	153	ARG
1	R	14	LEU
1	R	66	LEU
1	R	67	ASP
1	R	73	LEU
1	R	77	LEU
1	R	96	GLN
1	R	153	ARG
1	S	15	LEU
1	S	66	LEU
1	S	67	ASP
1	S	73	LEU
1	S	77	LEU
1	S	96	GLN
1	S	153	ARG

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Mol	Chain	Res	Type
1	T	13	ASN
1	T	66	LEU
1	T	67	ASP
1	T	73	LEU
1	T	77	LEU
1	T	96	GLN
1	T	153	ARG
1	U	13	ASN
1	U	23	ASP
1	U	66	LEU
1	U	67	ASP
1	U	73	LEU
1	U	77	LEU
1	U	96	GLN
1	U	111	ILE
1	U	153	ARG
1	V	23	ASP
1	V	66	LEU
1	V	67	ASP
1	V	73	LEU
1	V	77	LEU
1	V	96	GLN
1	V	102	THR
1	V	153	ARG
1	W	66	LEU
1	W	67	ASP
1	W	73	LEU
1	W	77	LEU
1	W	96	GLN
1	W	99	ASN
1	W	153	ARG
1	X	66	LEU
1	X	67	ASP
1	X	73	LEU
1	X	77	LEU
1	X	96	GLN
1	X	102	THR
1	X	153	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	36	GLN
1	A	63	HIS
1	A	86	GLN
1	A	96	GLN
1	B	36	GLN
1	B	63	HIS
1	B	86	GLN
1	B	96	GLN
1	B	99	ASN
1	C	36	GLN
1	C	86	GLN
1	C	96	GLN
1	D	36	GLN
1	D	63	HIS
1	D	86	GLN
1	D	96	GLN
1	E	36	GLN
1	E	51	HIS
1	E	63	HIS
1	E	86	GLN
1	E	96	GLN
1	F	13	ASN
1	F	36	GLN
1	F	63	HIS
1	F	86	GLN
1	F	96	GLN
1	F	99	ASN
1	G	36	GLN
1	G	63	HIS
1	G	86	GLN
1	G	96	GLN
1	G	99	ASN
1	H	36	GLN
1	H	63	HIS
1	H	86	GLN
1	H	96	GLN
1	H	99	ASN
1	I	36	GLN
1	I	63	HIS
1	I	86	GLN
1	I	96	GLN
1	I	99	ASN

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Mol	Chain	Res	Type
1	J	36	GLN
1	J	63	HIS
1	J	86	GLN
1	J	96	GLN
1	K	36	GLN
1	K	86	GLN
1	K	96	GLN
1	K	99	ASN
1	L	36	GLN
1	L	86	GLN
1	L	96	GLN
1	L	99	ASN
1	L	115	GLN
1	M	36	GLN
1	M	51	HIS
1	M	63	HIS
1	M	86	GLN
1	M	96	GLN
1	M	99	ASN
1	N	13	ASN
1	N	36	GLN
1	N	51	HIS
1	N	63	HIS
1	N	86	GLN
1	N	96	GLN
1	O	13	ASN
1	O	36	GLN
1	O	51	HIS
1	O	63	HIS
1	O	96	GLN
1	O	99	ASN
1	P	36	GLN
1	P	86	GLN
1	P	96	GLN
1	Q	36	GLN
1	Q	63	HIS
1	Q	86	GLN
1	Q	96	GLN
1	Q	99	ASN
1	R	13	ASN
1	R	36	GLN
1	R	63	HIS

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Mol	Chain	Res	Type
1	R	86	GLN
1	R	96	GLN
1	R	99	ASN
1	S	36	GLN
1	S	63	HIS
1	S	86	GLN
1	S	96	GLN
1	S	99	ASN
1	S	115	GLN
1	T	36	GLN
1	T	63	HIS
1	T	86	GLN
1	T	96	GLN
1	T	113	ASN
1	U	13	ASN
1	U	36	GLN
1	U	63	HIS
1	U	86	GLN
1	U	96	GLN
1	V	36	GLN
1	V	63	HIS
1	V	86	GLN
1	V	96	GLN
1	W	13	ASN
1	W	36	GLN
1	W	63	HIS
1	W	86	GLN
1	W	96	GLN
1	X	36	GLN
1	X	63	HIS
1	X	86	GLN
1	X	96	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TRS	A	301	-	7,7,7	0.64	0	9,9,9	1.36	2 (22%)
2	TRS	A	309	-	7,7,7	0.87	1 (14%)	9,9,9	1.52	2 (22%)
2	TRS	C	307	-	7,7,7	0.58	0	9,9,9	1.40	2 (22%)
2	TRS	D	305	-	7,7,7	0.70	0	9,9,9	1.49	2 (22%)
2	TRS	D	306	-	7,7,7	0.65	0	9,9,9	1.46	2 (22%)
2	TRS	D	310	-	7,7,7	0.66	0	9,9,9	1.55	2 (22%)
2	TRS	E	312	-	7,7,7	0.77	0	9,9,9	1.45	2 (22%)
2	TRS	G	302	-	7,7,7	0.86	0	9,9,9	1.39	2 (22%)
2	TRS	G	303	-	7,7,7	0.67	0	9,9,9	1.55	2 (22%)
2	TRS	H	304	-	7,7,7	0.75	0	9,9,9	1.38	2 (22%)
2	TRS	H	308	-	7,7,7	0.73	0	9,9,9	1.50	2 (22%)
2	TRS	L	311	-	7,7,7	0.66	0	9,9,9	1.42	2 (22%)
2	TRS	M	313	-	7,7,7	0.37	0	9,9,9	1.47	2 (22%)
2	TRS	M	321	-	7,7,7	0.61	0	9,9,9	1.25	1 (11%)
2	TRS	P	317	-	7,7,7	0.65	0	9,9,9	1.45	2 (22%)
2	TRS	P	318	-	7,7,7	0.83	0	9,9,9	1.51	2 (22%)
2	TRS	P	322	-	7,7,7	0.49	0	9,9,9	1.61	2 (22%)
2	TRS	Q	324	-	7,7,7	0.64	0	9,9,9	1.46	2 (22%)
2	TRS	R	319	-	7,7,7	0.35	0	9,9,9	1.47	2 (22%)
2	TRS	T	316	-	7,7,7	0.59	0	9,9,9	1.38	2 (22%)
2	TRS	T	320	-	7,7,7	0.70	0	9,9,9	1.45	2 (22%)
2	TRS	W	314	-	7,7,7	0.93	0	9,9,9	1.45	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRS	W	315	-	7,7,7	0.59	0	9,9,9	1.38	2 (22%)
2	TRS	X	323	-	7,7,7	0.71	0	9,9,9	1.42	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	A	301	-	-	0/9/9/9	0/0/0/0
2	TRS	A	309	-	-	0/9/9/9	0/0/0/0
2	TRS	C	307	-	-	0/9/9/9	0/0/0/0
2	TRS	D	305	-	-	0/9/9/9	0/0/0/0
2	TRS	D	306	-	-	0/9/9/9	0/0/0/0
2	TRS	D	310	-	-	0/9/9/9	0/0/0/0
2	TRS	E	312	-	-	0/9/9/9	0/0/0/0
2	TRS	G	302	-	-	0/9/9/9	0/0/0/0
2	TRS	G	303	-	-	0/9/9/9	0/0/0/0
2	TRS	H	304	-	-	0/9/9/9	0/0/0/0
2	TRS	H	308	-	-	0/9/9/9	0/0/0/0
2	TRS	L	311	-	-	0/9/9/9	0/0/0/0
2	TRS	M	313	-	-	0/9/9/9	0/0/0/0
2	TRS	M	321	-	-	0/9/9/9	0/0/0/0
2	TRS	P	317	-	-	0/9/9/9	0/0/0/0
2	TRS	P	318	-	-	0/9/9/9	0/0/0/0
2	TRS	P	322	-	-	0/9/9/9	0/0/0/0
2	TRS	Q	324	-	-	0/9/9/9	0/0/0/0
2	TRS	R	319	-	-	0/9/9/9	0/0/0/0
2	TRS	T	316	-	-	0/9/9/9	0/0/0/0
2	TRS	T	320	-	-	0/9/9/9	0/0/0/0
2	TRS	W	314	-	-	0/9/9/9	0/0/0/0
2	TRS	W	315	-	-	0/9/9/9	0/0/0/0
2	TRS	X	323	-	-	0/9/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	309	TRS	C-N	-2.06	1.47	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	309	TRS	C1-C-N	-3.17	102.32	108.09
2	G	303	TRS	C1-C-N	-3.04	102.56	108.09
2	D	305	TRS	C1-C-N	-2.97	102.69	108.09
2	P	318	TRS	C1-C-N	-2.96	102.70	108.09
2	D	306	TRS	C1-C-N	-2.94	102.73	108.09
2	Q	324	TRS	C1-C-N	-2.92	102.77	108.09
2	E	312	TRS	C1-C-N	-2.89	102.83	108.09
2	P	317	TRS	C1-C-N	-2.86	102.89	108.09
2	W	314	TRS	C1-C-N	-2.85	102.89	108.09
2	H	308	TRS	C1-C-N	-2.84	102.91	108.09
2	T	320	TRS	C1-C-N	-2.81	102.97	108.09
2	X	323	TRS	C1-C-N	-2.76	103.07	108.09
2	L	311	TRS	C1-C-N	-2.72	103.14	108.09
2	D	310	TRS	C1-C-N	-2.70	103.18	108.09
2	G	302	TRS	C1-C-N	-2.69	103.20	108.09
2	P	322	TRS	C1-C-N	-2.59	103.37	108.09
2	R	319	TRS	C1-C-N	-2.58	103.39	108.09
2	W	315	TRS	C1-C-N	-2.58	103.40	108.09
2	T	316	TRS	C1-C-N	-2.51	103.52	108.09
2	A	301	TRS	C1-C-N	-2.46	103.61	108.09
2	H	304	TRS	C1-C-N	-2.34	103.83	108.09
2	M	321	TRS	C1-C-N	-2.30	103.90	108.09
2	M	313	TRS	C1-C-N	-2.12	104.23	108.09
2	C	307	TRS	C1-C-N	-2.05	104.35	108.09
2	E	312	TRS	C3-C-N	2.20	112.09	108.09
2	A	309	TRS	C3-C-N	2.20	112.09	108.09
2	W	315	TRS	C3-C-N	2.24	112.17	108.09
2	A	301	TRS	C3-C-N	2.27	112.23	108.09
2	H	304	TRS	C3-C-N	2.31	112.30	108.09
2	X	323	TRS	C3-C-N	2.33	112.32	108.09
2	D	306	TRS	C3-C-N	2.36	112.38	108.09
2	L	311	TRS	C3-C-N	2.39	112.44	108.09
2	P	318	TRS	C3-C-N	2.44	112.53	108.09
2	G	302	TRS	C3-C-N	2.47	112.58	108.09
2	T	316	TRS	C3-C-N	2.49	112.62	108.09
2	W	314	TRS	C3-C-N	2.50	112.63	108.09
2	D	305	TRS	C3-C-N	2.50	112.64	108.09
2	Q	324	TRS	C3-C-N	2.56	112.75	108.09
2	T	320	TRS	C3-C-N	2.57	112.76	108.09
2	P	317	TRS	C3-C-N	2.57	112.77	108.09
2	R	319	TRS	C3-C-N	2.61	112.84	108.09
2	C	307	TRS	C3-C-N	2.62	112.85	108.09
2	M	313	TRS	C3-C-N	2.63	112.88	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	303	TRS	C3-C-N	2.64	112.89	108.09
2	H	308	TRS	C3-C-N	2.69	112.98	108.09
2	D	310	TRS	C3-C-N	2.83	113.24	108.09
2	P	322	TRS	C3-C-N	2.91	113.39	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	312	TRS	1	0
2	G	303	TRS	1	0
2	P	318	TRS	1	0
2	Q	324	TRS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	155/167 (92%)	-0.25	1 (0%) 90 88	39, 59, 80, 85	0
1	B	155/167 (92%)	-0.20	0 100 100	39, 63, 78, 86	0
1	C	154/167 (92%)	-0.10	3 (1%) 70 64	42, 65, 84, 95	0
1	D	154/167 (92%)	-0.05	6 (3%) 43 35	34, 62, 91, 96	0
1	E	156/167 (93%)	-0.33	0 100 100	36, 59, 78, 88	0
1	F	155/167 (92%)	-0.38	3 (1%) 70 64	35, 57, 86, 98	0
1	G	155/167 (92%)	0.19	2 (1%) 79 75	54, 81, 100, 108	0
1	H	154/167 (92%)	0.05	5 (3%) 51 44	45, 71, 95, 100	0
1	I	154/167 (92%)	-0.39	0 100 100	33, 59, 78, 83	0
1	J	158/167 (94%)	-0.11	2 (1%) 79 75	47, 67, 82, 107	0
1	K	154/167 (92%)	0.04	5 (3%) 51 44	53, 75, 90, 94	0
1	L	155/167 (92%)	-0.01	1 (0%) 90 88	49, 74, 90, 95	0
1	M	156/167 (93%)	-0.29	2 (1%) 79 75	30, 59, 82, 96	0
1	N	156/167 (93%)	-0.58	2 (1%) 79 75	29, 50, 68, 88	0
1	O	156/167 (93%)	-0.31	0 100 100	39, 62, 79, 97	0
1	P	154/167 (92%)	-0.32	2 (1%) 79 75	38, 57, 78, 85	0
1	Q	154/167 (92%)	-0.10	2 (1%) 79 75	37, 65, 85, 89	0
1	R	156/167 (93%)	-0.24	2 (1%) 79 75	40, 59, 83, 89	0
1	S	156/167 (93%)	-0.50	0 100 100	36, 54, 69, 80	0
1	T	156/167 (93%)	-0.50	0 100 100	23, 46, 66, 84	0
1	U	157/167 (94%)	-0.24	1 (0%) 90 88	38, 61, 78, 89	0
1	V	155/167 (92%)	-0.41	3 (1%) 70 64	32, 50, 70, 77	0
1	W	156/167 (93%)	-0.47	0 100 100	29, 48, 66, 79	0
1	X	156/167 (93%)	-0.41	2 (1%) 79 75	30, 49, 78, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3727/4008 (92%)	-0.25	44 (1%) 81 77	23, 61, 87, 108	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	12	THR	4.3
1	X	13	ASN	3.9
1	R	12	THR	3.6
1	G	14	LEU	3.4
1	K	140	LYS	3.3
1	H	92	LEU	3.2
1	V	14	LEU	3.2
1	D	140	LYS	3.1
1	X	12	THR	3.1
1	F	14	LEU	2.9
1	J	11	ALA	2.9
1	K	138	GLU	2.9
1	C	134	LYS	2.7
1	F	13	ASN	2.6
1	C	140	LYS	2.6
1	K	167	GLU	2.6
1	Q	24	SER	2.6
1	A	13	ASN	2.5
1	V	13	ASN	2.5
1	H	24	SER	2.4
1	P	14	LEU	2.4
1	F	24	SER	2.4
1	C	24	SER	2.4
1	N	13	ASN	2.4
1	V	140	LYS	2.4
1	D	16	TYR	2.3
1	H	25	GLU	2.3
1	D	24	SER	2.3
1	U	140	LYS	2.3
1	D	27	LYS	2.2
1	M	31	GLU	2.1
1	D	17	THR	2.1
1	Q	136	ILE	2.1
1	G	112	HIS	2.1
1	M	13	ASN	2.1
1	R	13	ASN	2.1
1	H	134	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	25	GLU	2.1
1	K	99	ASN	2.1
1	D	31	GLU	2.1
1	K	15	LEU	2.0
1	J	134	LYS	2.0
1	H	21	VAL	2.0
1	P	24	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TRS	G	303	8/8	0.81	0.41	1.72	101,104,104,105	0
2	TRS	T	316	8/8	0.95	0.15	1.26	51,53,56,57	0
2	TRS	A	301	8/8	0.92	0.13	1.07	54,56,57,59	0
2	TRS	C	307	8/8	0.94	0.15	1.03	51,52,53,54	0
2	TRS	P	322	8/8	0.96	0.13	0.43	44,46,47,48	0
2	TRS	R	319	8/8	0.95	0.13	0.19	45,50,53,56	0
2	TRS	Q	324	8/8	0.92	0.18	-0.15	67,69,70,71	0
2	TRS	D	306	8/8	0.91	0.16	-0.23	65,68,69,70	0
2	TRS	A	309	8/8	0.93	0.17	-0.57	58,61,61,62	0
2	TRS	D	310	8/8	0.91	0.13	-0.59	64,64,65,66	0
2	TRS	M	321	8/8	0.94	0.10	-1.17	54,55,56,57	0
2	TRS	P	318	8/8	0.89	0.13	-1.24	64,69,70,72	0
2	TRS	M	313	8/8	0.95	0.10	-1.25	48,50,51,52	0
2	TRS	W	315	8/8	0.92	0.12	-1.60	87,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	TRS	H	304	8/8	0.94	0.10	-1.67	54,56,58,59	0
2	TRS	E	312	8/8	0.90	0.12	-1.80	73,75,76,76	0
2	TRS	P	317	8/8	0.76	0.30	-	87,88,89,92	0
2	TRS	D	305	8/8	0.84	0.25	-	83,83,85,86	0
2	TRS	G	302	8/8	0.77	0.33	-	105,106,107,108	0
2	TRS	L	311	8/8	0.90	0.19	-	74,75,76,77	0
2	TRS	T	320	8/8	0.84	0.24	-	86,87,88,89	0
2	TRS	H	308	8/8	0.80	0.29	-	86,88,89,91	0
2	TRS	X	323	8/8	0.86	0.23	-	82,83,85,85	0
2	TRS	W	314	8/8	0.87	0.18	-	68,69,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.