Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 02:34 PM EST

PDB ID	:	4E2I
Title	:	The Complex Structure of the SV40 Helicase Large T Antigen and p68 Subunit of DNA Polymerase Alpha-Primase
Authors	:	Zhou, B.; Arnett, D.R.; Yu, X.; Brewster, A.; Sowd, G.A.; Xie, C.L.; Vila, S.; Gai, D.; Fanning, E.; Chen, X.S.
Deposited on	:	2012-03-08
Resolution	:	5.00 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

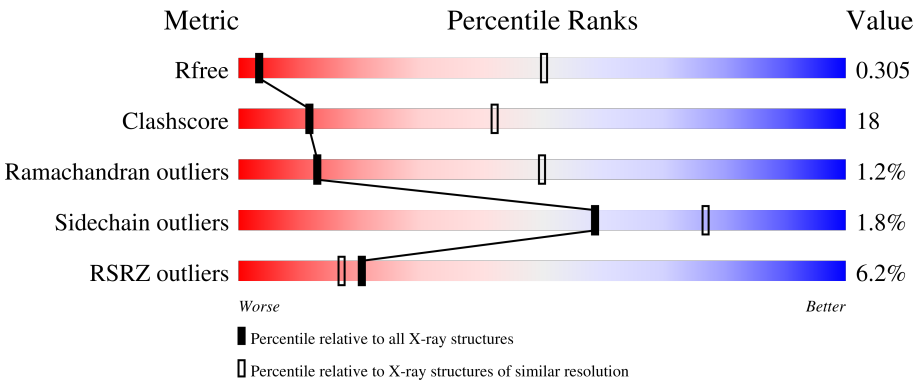
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1140 (6.20-3.80)
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)
RSRZ outliers	127900	1010 (6.22-3.72)

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

Mol	Chain	Length	Quality of chain
1	A	362	6% 61% 38%
1	B	362	2% 62% 36%
1	C	362	2% 62% 37%
1	D	362	2% 59% 39%
1	E	362	2% 61% 37%

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Mol	Chain	Length	Quality of chain
1	F	362	2% 60% 38%
1	G	362	6% 61% 37%
1	H	362	3% 63% 36%
1	I	362	4% 59% 39%
1	J	362	3% 60% 38%
1	K	362	2% 60% 38%
1	L	362	4% 60% 39%
2	1	78	24% 54% 44%
2	2	78	13% 55% 44%
2	3	78	17% 54% 44%
2	4	78	31% 56% 41%
2	5	78	24% 55% 42%
2	6	78	22% 55% 42%
2	7	78	15% 55% 42%
2	8	78	31% 55% 42%
2	9	78	22% 54% 44%
2	U	78	23% 53% 45%
2	W	78	12% 55% 42%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 41874 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 Large T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	362	2933	1888	493	531	21	0	0	0
1	B	362	2933	1888	493	531	21	0	0	0
1	C	362	2933	1888	493	531	21	0	0	0
1	D	362	2933	1888	493	531	21	0	0	0
1	E	362	2933	1888	493	531	21	0	0	0
1	F	362	2933	1888	493	531	21	0	0	0
1	G	362	2933	1888	493	531	21	0	0	0
1	H	362	2933	1888	493	531	21	0	0	0
1	I	362	2933	1888	493	531	21	0	0	0
1	J	362	2933	1888	493	531	21	0	0	0
1	K	362	2933	1888	493	531	21	0	0	0
1	L	362	2933	1888	493	531	21	0	0	0

- Molecule 2 is a protein called DNA polymerase alpha subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	78	606	380	99	122	5	0	0	0
2	3	78	606	380	99	122	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	6	78	606	380	99	122	5	0	0	0
2	U	78	606	380	99	122	5	0	0	0
2	W	78	606	380	99	122	5	0	0	0
2	5	78	606	380	99	122	5	0	0	0
2	7	78	606	380	99	122	5	0	0	0
2	9	78	606	380	99	122	5	0	0	0
2	1	78	606	380	99	122	5	0	0	0
2	4	78	606	380	99	122	5	0	0	0
2	8	78	606	380	99	122	5	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0
3	E	1	1	1	0	0
3	F	1	1	1	0	0
3	G	1	1	1	0	0
3	H	1	1	1	0	0
3	I	1	1	1	0	0
3	J	1	1	1	0	0

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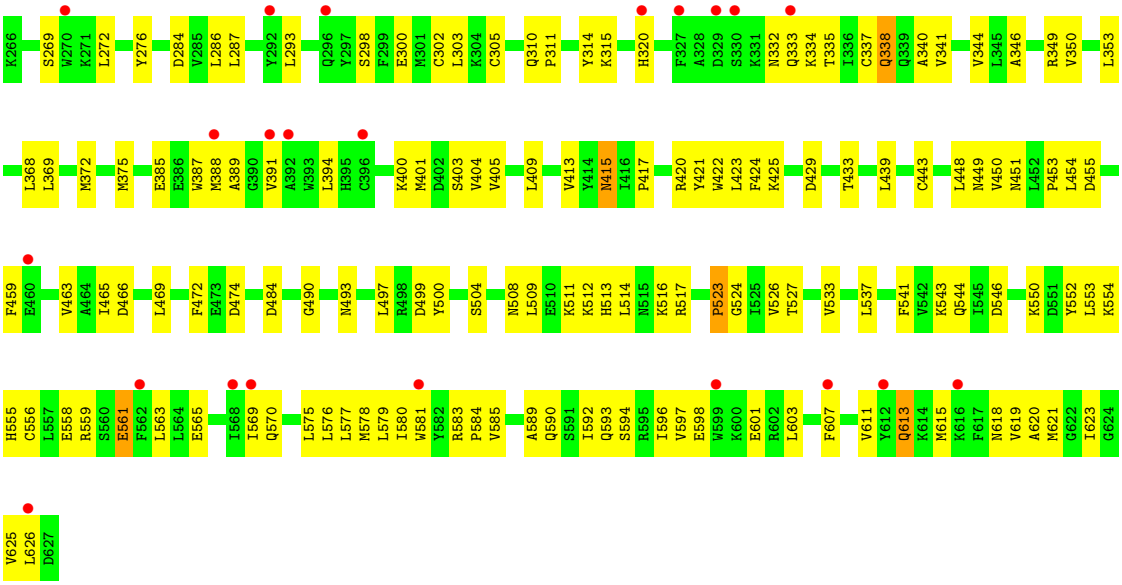
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	K	1	1	1	0	0
			Total	Zn		
3	L	1	1	1	0	0

3 Residue-property plots (i)

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

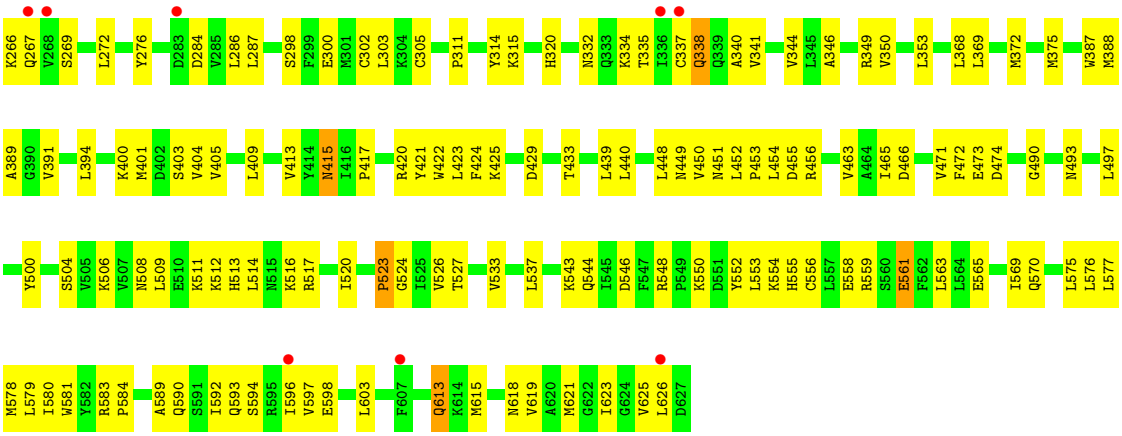
• Molecule 1: Large T antigen

Chain A: 6% 61% 38%



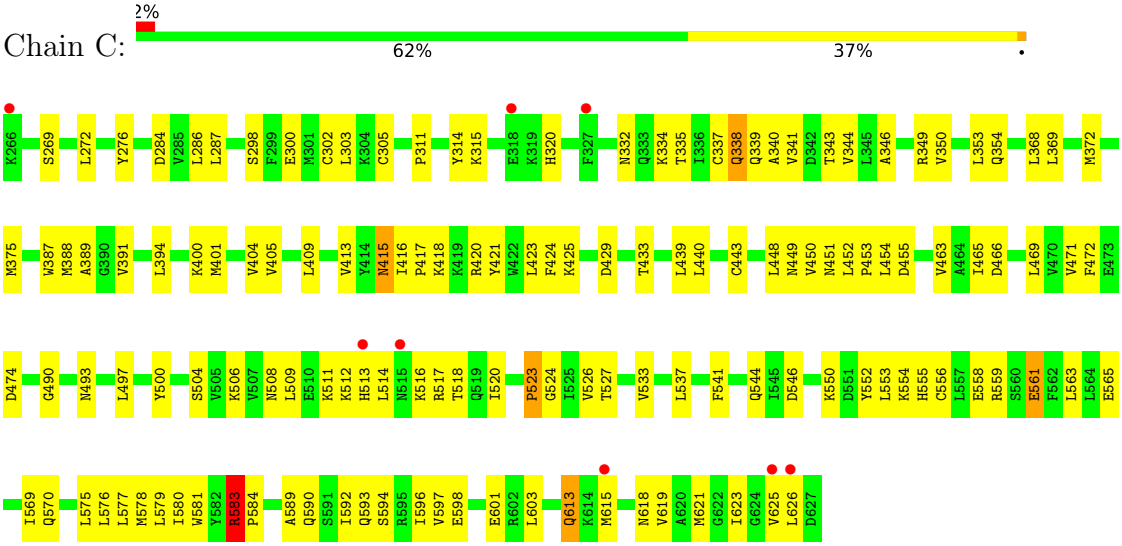
• Molecule 1: Large T antigen

Chain B: 2% 62% 36%



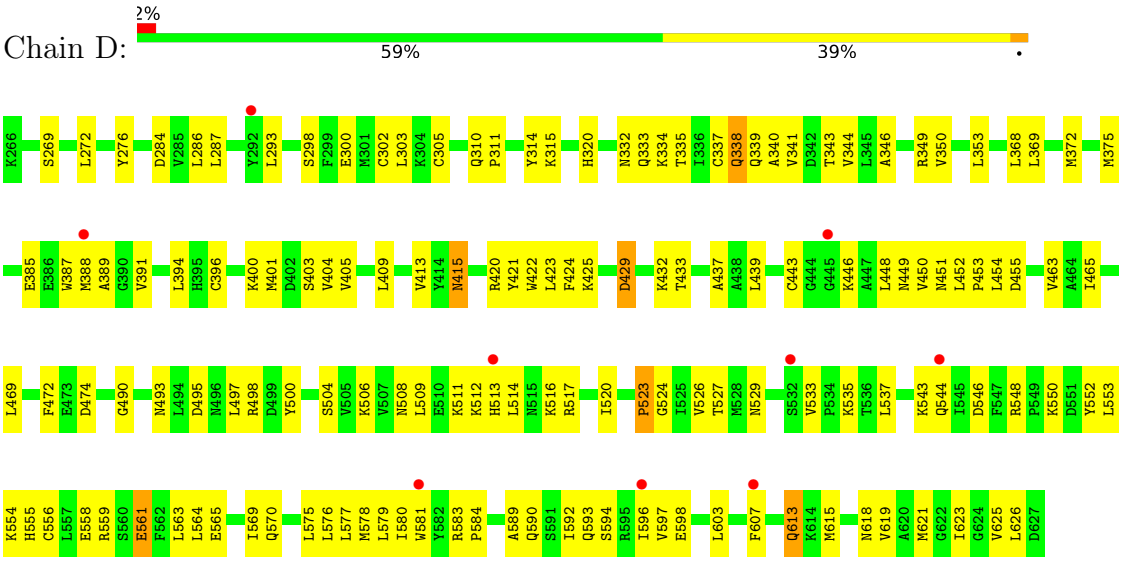
• Molecule 1: Large T antigen

Chain C:



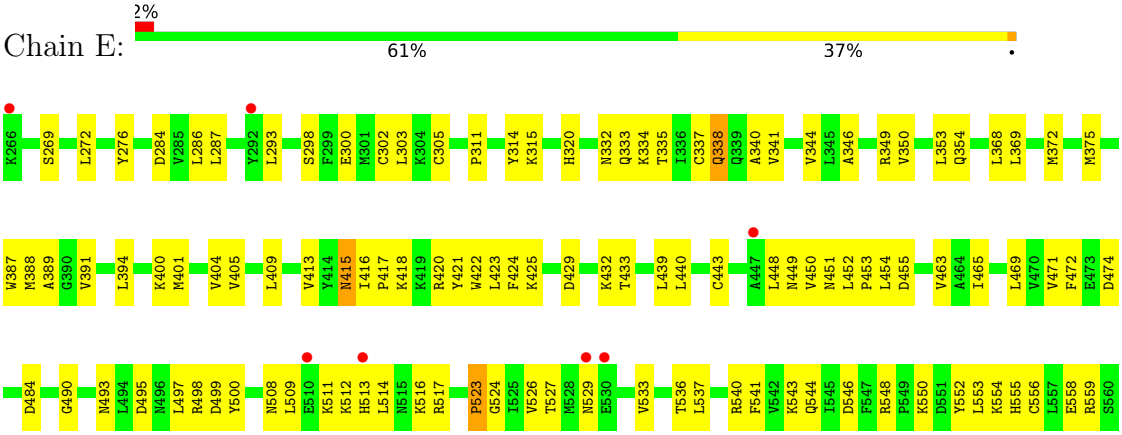
• Molecule 1: Large T antigen

Chain D:



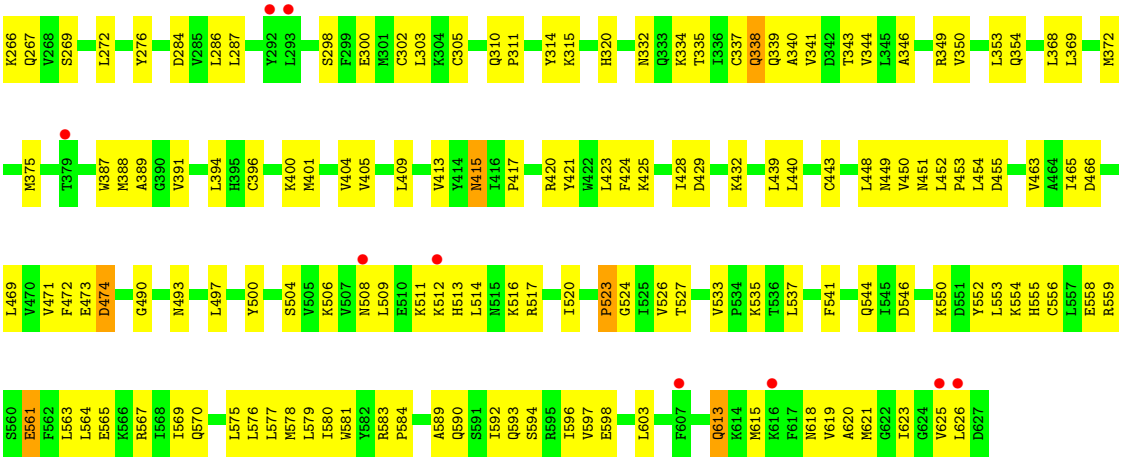
• Molecule 1: Large T antigen

Chain E:



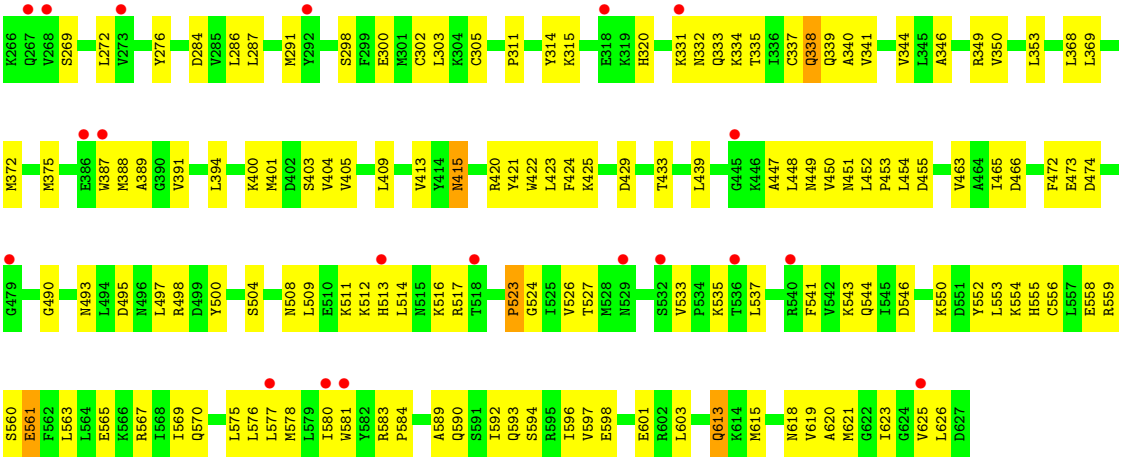
• Molecule 1: Large T antigen

Chain F:



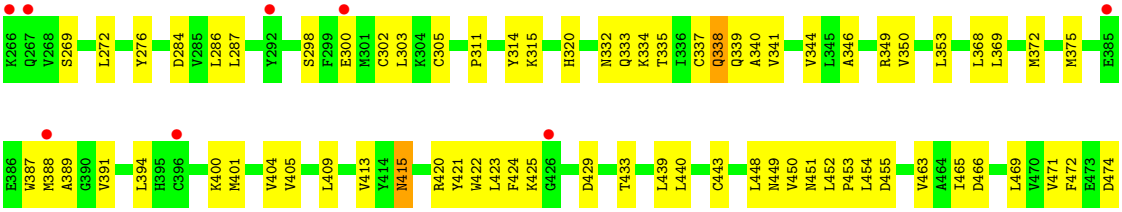
• Molecule 1: Large T antigen

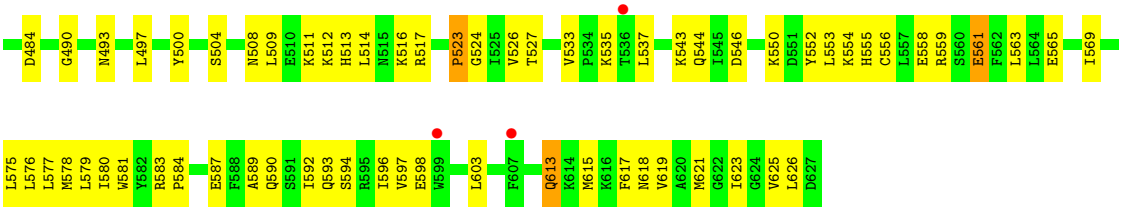
Chain G:



• Molecule 1: Large T antigen

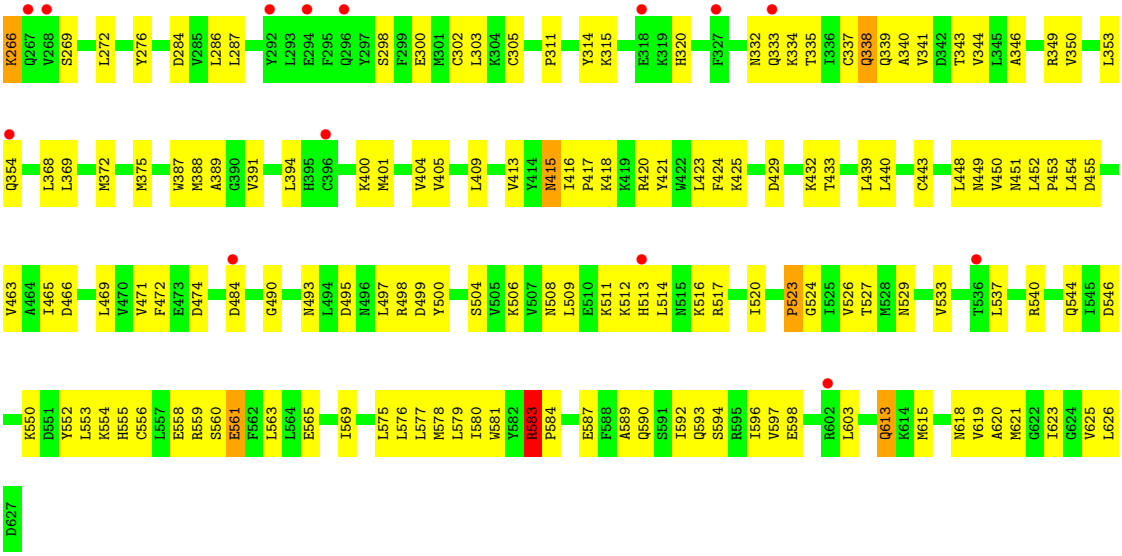
Chain H:





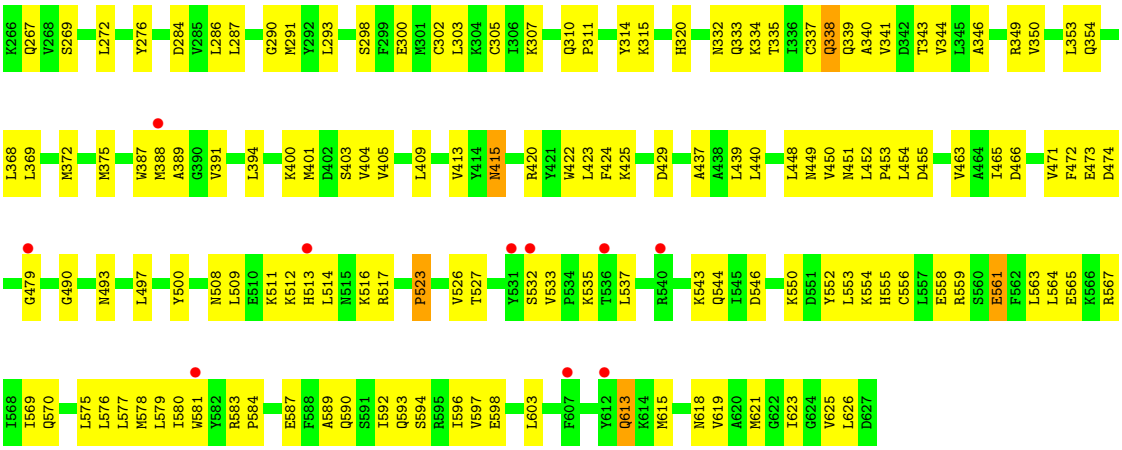
- Molecule 1: Large T antigen

Chain I:



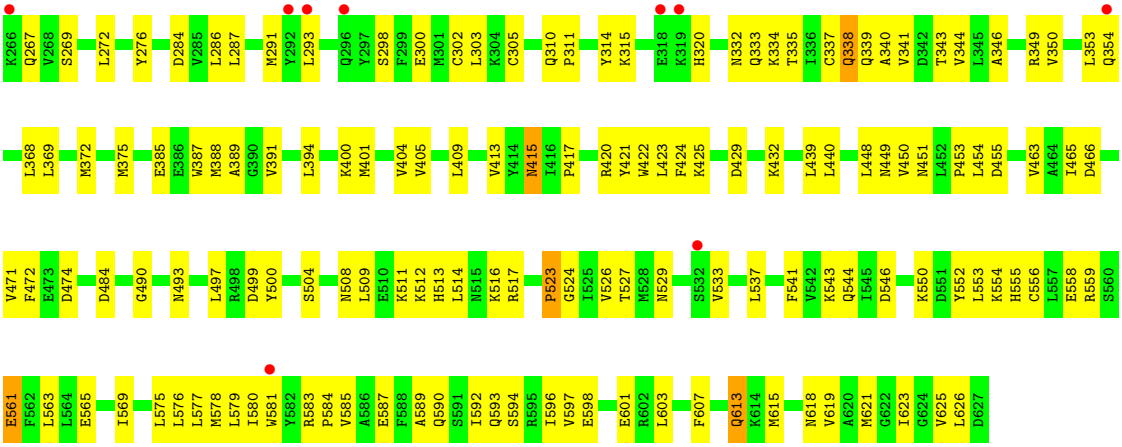
- Molecule 1: Large T antigen

Chain J:



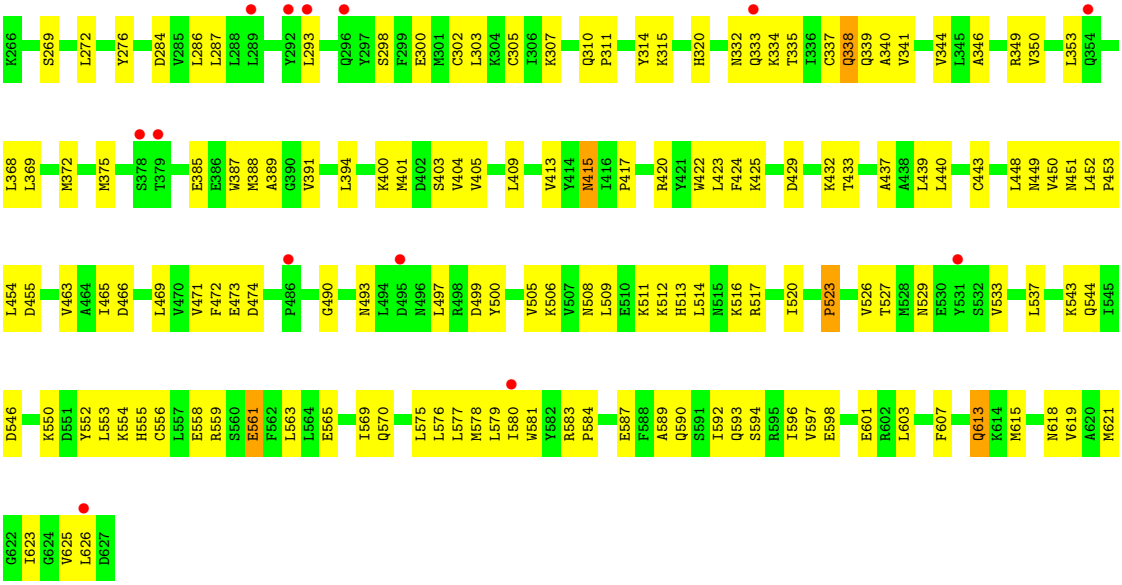
- Molecule 1: Large T antigen

Chain K:



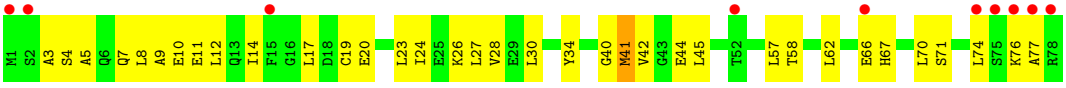
- Molecule 1: Large T antigen

Chain L:



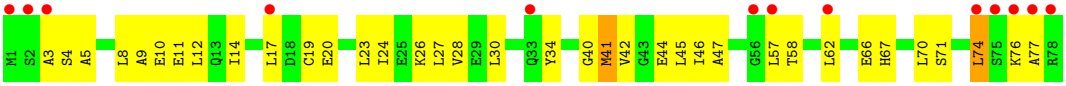
- Molecule 2: DNA polymerase alpha subunit B

Chain 2:



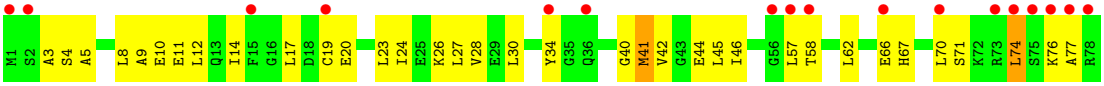
- Molecule 2: DNA polymerase alpha subunit B

Chain 3:



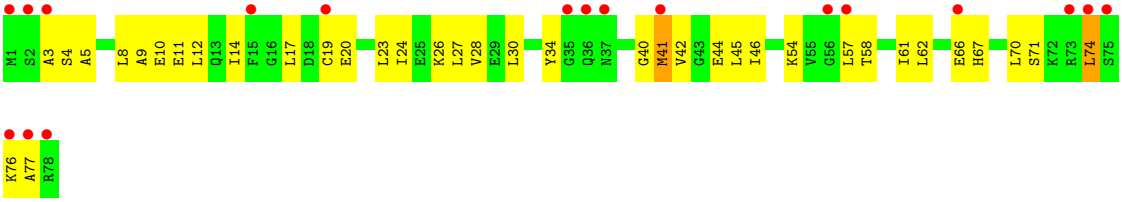
• Molecule 2: DNA polymerase alpha subunit B

Chain 6:



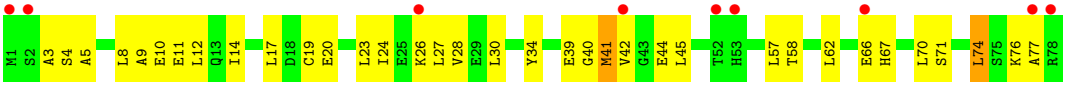
• Molecule 2: DNA polymerase alpha subunit B

Chain U:



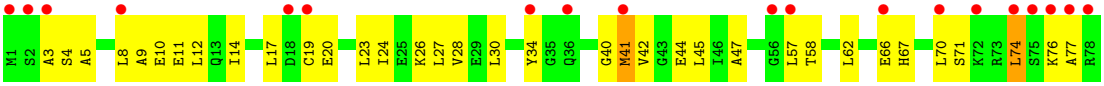
• Molecule 2: DNA polymerase alpha subunit B

Chain W:



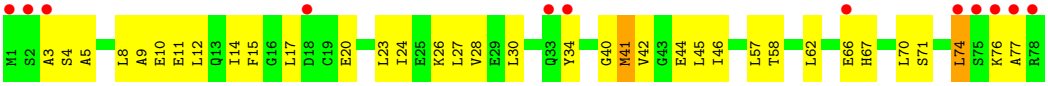
• Molecule 2: DNA polymerase alpha subunit B

Chain 5:



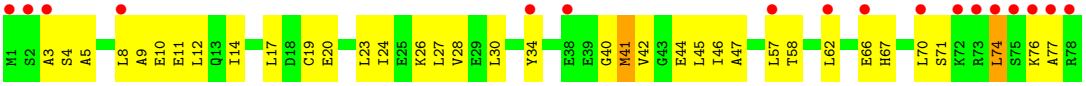
• Molecule 2: DNA polymerase alpha subunit B

Chain 7:



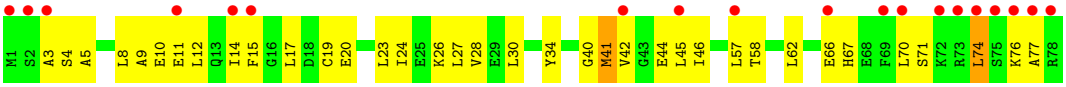
• Molecule 2: DNA polymerase alpha subunit B

Chain 9:



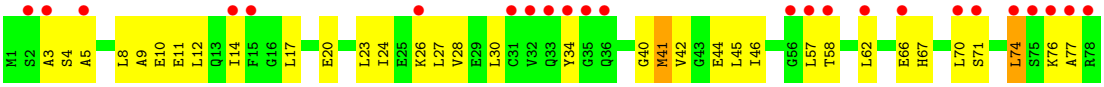
• Molecule 2: DNA polymerase alpha subunit B

Chain 1:



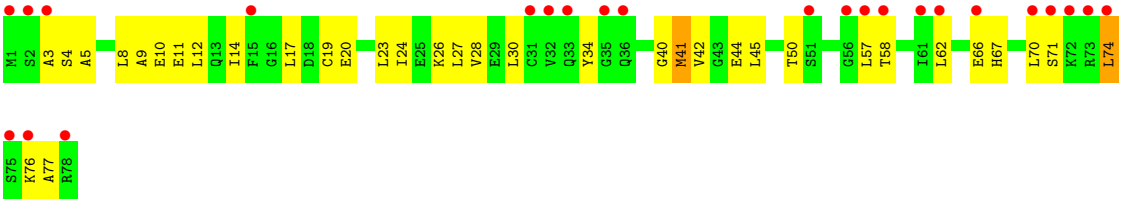
• Molecule 2: DNA polymerase alpha subunit B

Chain 4:



• Molecule 2: DNA polymerase alpha subunit B

Chain 8:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	249.10Å 249.10Å 387.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 5.00 49.91 – 5.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-5.00) 74.4 (49.91-5.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 5.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.305 , 0.314 0.299 , 0.305	Depositor DCC
R_{free} test set	2006 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	280.1	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 273.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	41874	wwPDB-VP
Average B, all atoms (Å^2)	299.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.25	0/2992	0.43	0/4030
1	B	0.25	0/2992	0.43	0/4030
1	C	0.26	0/2992	0.63	3/4030 (0.1%)
1	D	0.25	0/2992	0.43	0/4030
1	E	0.25	0/2992	0.43	0/4030
1	F	0.25	0/2992	0.43	0/4030
1	G	0.25	0/2992	0.43	0/4030
1	H	0.25	0/2992	0.43	0/4030
1	I	0.26	0/2992	0.63	3/4030 (0.1%)
1	J	0.25	0/2992	0.43	0/4030
1	K	0.25	0/2992	0.43	0/4030
1	L	0.24	0/2992	0.43	0/4030
2	1	0.25	0/612	0.43	0/820
2	2	0.26	0/612	0.44	0/820
2	3	0.25	0/612	0.43	0/820
2	4	0.25	0/612	0.44	0/820
2	5	0.26	0/612	0.43	0/820
2	6	0.26	0/612	0.44	0/820
2	7	0.25	0/612	0.43	0/820
2	8	0.25	0/612	0.43	0/820
2	9	0.26	0/612	0.43	0/820
2	U	0.25	0/612	0.43	0/820
2	W	0.26	0/612	0.44	0/820
All	All	0.25	0/42636	0.46	6/57380 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	583	ARG	NE-CZ-NH1	-20.00	110.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	583	ARG	NE-CZ-NH1	-19.96	110.32	120.30
1	I	583	ARG	NE-CZ-NH2	19.44	130.02	120.30
1	C	583	ARG	NE-CZ-NH2	19.40	130.00	120.30
1	C	583	ARG	CD-NE-CZ	8.62	135.67	123.60
1	I	583	ARG	CD-NE-CZ	8.61	135.65	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2984	105	0
1	B	2933	0	2984	101	0
1	C	2933	0	2984	103	0
1	D	2933	0	2984	112	0
1	E	2933	0	2984	105	0
1	F	2933	0	2984	116	0
1	G	2933	0	2984	112	0
1	H	2933	0	2984	97	0
1	I	2933	0	2984	116	0
1	J	2933	0	2984	112	0
1	K	2933	0	2984	111	0
1	L	2933	0	2984	125	0
2	1	606	0	602	29	0
2	2	606	0	602	30	0
2	3	606	0	602	28	0
2	4	606	0	602	30	0
2	5	606	0	602	27	0
2	6	606	0	602	34	0
2	7	606	0	602	28	0
2	8	606	0	602	27	0
2	9	606	0	602	29	0
2	U	606	0	602	30	0
2	W	606	0	602	28	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	41874	0	42430	1479	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 18.

All (1479) 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:G:286:LEU:HD12	1:L:349:ARG:HH21	1.16	1.07
1:J:349:ARG:HH21	1:K:286:LEU:HD12	1.30	0.97
1:D:349:ARG:HH21	1:E:286:LEU:HD12	1.30	0.96
1:H:349:ARG:HH21	1:I:286:LEU:HD12	1.35	0.92
1:K:349:ARG:HH21	1:L:286:LEU:HD12	1.38	0.89
1:E:349:ARG:HH21	1:F:286:LEU:HD12	1.40	0.86
1:A:286:LEU:HD12	1:F:349:ARG:HH21	1.41	0.85
1:G:349:ARG:HH21	1:H:286:LEU:HD12	1.44	0.79
1:I:349:ARG:HH21	1:J:286:LEU:HD12	1.50	0.77
1:J:339:GLN:NE2	1:K:333:GLN:H	1.83	0.76
1:I:621:MET:HE1	2:9:46:ILE:HB	1.68	0.76
1:A:298:SER:HB2	1:A:300:GLU:HG2	1.68	0.76
1:D:298:SER:HB2	1:D:300:GLU:HG2	1.69	0.74
1:I:298:SER:HB2	1:I:300:GLU:HG2	1.69	0.74
1:F:396:CYS:HA	2:6:14:ILE:CG2	2.16	0.74
1:H:298:SER:HB2	1:H:300:GLU:HG2	1.69	0.74
1:C:298:SER:HB2	1:C:300:GLU:HG2	1.70	0.74
1:J:298:SER:HB2	1:J:300:GLU:HG2	1.69	0.74
1:B:298:SER:HB2	1:B:300:GLU:HG2	1.70	0.74
1:F:298:SER:HB2	1:F:300:GLU:HG2	1.69	0.73
1:G:298:SER:HB2	1:G:300:GLU:HG2	1.70	0.73
1:C:305:CYS:HA	1:C:314:TYR:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:298:SER:HB2	1:L:300:GLU:HG2	1.69	0.73
1:I:417:PRO:HG2	1:J:570:GLN:HE21	1.53	0.73
1:K:305:CYS:HA	1:K:314:TYR:HB3	1.71	0.73
1:H:305:CYS:HA	1:H:314:TYR:HB3	1.71	0.73
1:I:416:ILE:HG23	1:J:564:LEU:HB3	1.69	0.73
1:K:298:SER:HB2	1:K:300:GLU:HG2	1.69	0.72
1:B:305:CYS:HA	1:B:314:TYR:HB3	1.71	0.72
1:E:298:SER:HB2	1:E:300:GLU:HG2	1.69	0.72
1:J:305:CYS:HA	1:J:314:TYR:HB3	1.71	0.72
1:E:305:CYS:HA	1:E:314:TYR:HB3	1.71	0.72
1:A:305:CYS:HA	1:A:314:TYR:HB3	1.71	0.71
1:F:305:CYS:HA	1:F:314:TYR:HB3	1.71	0.71
1:I:305:CYS:HA	1:I:314:TYR:HB3	1.71	0.71
1:I:354:GLN:HG2	1:J:310:GLN:HG3	1.71	0.71
1:L:305:CYS:HA	1:L:314:TYR:HB3	1.71	0.71
1:D:305:CYS:HA	1:D:314:TYR:HB3	1.71	0.70
1:G:305:CYS:HA	1:G:314:TYR:HB3	1.71	0.70
1:A:349:ARG:HH21	1:B:286:LEU:HD12	1.56	0.70
1:J:349:ARG:HH11	1:J:517:ARG:HD3	1.57	0.70
1:C:349:ARG:HH11	1:C:517:ARG:HD3	1.57	0.70
1:B:349:ARG:HH21	1:C:286:LEU:HD12	1.58	0.69
1:F:621:MET:HE1	2:6:46:ILE:HG22	1.75	0.69
1:D:349:ARG:HH11	1:D:517:ARG:HD3	1.57	0.69
1:H:349:ARG:HH11	1:H:517:ARG:HD3	1.57	0.69
1:A:349:ARG:HH11	1:A:517:ARG:HD3	1.57	0.69
1:E:349:ARG:HH11	1:E:517:ARG:HD3	1.57	0.69
1:K:424:PHE:HB2	1:K:527:THR:HG22	1.75	0.69
1:F:349:ARG:HH11	1:F:517:ARG:HD3	1.57	0.68
1:G:349:ARG:HH11	1:G:517:ARG:HD3	1.59	0.68
1:H:424:PHE:HB2	1:H:527:THR:HG22	1.75	0.68
1:L:349:ARG:HH11	1:L:517:ARG:HD3	1.58	0.68
1:A:424:PHE:HB2	1:A:527:THR:HG22	1.75	0.68
1:D:339:GLN:NE2	1:E:333:GLN:H	1.92	0.68
1:G:424:PHE:HB2	1:G:527:THR:HG22	1.75	0.68
1:H:535:LYS:HE2	1:I:484:ASP:HB2	1.75	0.68
1:L:563:LEU:HB3	1:L:569:ILE:HG23	1.76	0.68
1:B:424:PHE:HB2	1:B:527:THR:HG22	1.76	0.68
1:F:424:PHE:HB2	1:F:527:THR:HG22	1.75	0.68
1:D:424:PHE:HB2	1:D:527:THR:HG22	1.74	0.68
1:E:416:ILE:HG23	1:F:564:LEU:HB3	1.74	0.68
1:K:349:ARG:HH11	1:K:517:ARG:HD3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:349:ARG:HH11	1:I:517:ARG:HD3	1.57	0.68
1:L:424:PHE:HB2	1:L:527:THR:HG22	1.75	0.68
1:J:424:PHE:HB2	1:J:527:THR:HG22	1.76	0.68
1:I:424:PHE:HB2	1:I:527:THR:HG22	1.76	0.67
1:J:563:LEU:HB3	1:J:569:ILE:HG23	1.76	0.67
1:K:563:LEU:HB3	1:K:569:ILE:HG23	1.76	0.67
1:C:417:PRO:HG2	1:D:570:GLN:HE21	1.59	0.67
1:C:563:LEU:HB3	1:C:569:ILE:HG23	1.76	0.67
1:A:563:LEU:HB3	1:A:569:ILE:HG23	1.77	0.67
1:E:417:PRO:HG2	1:F:570:GLN:HE21	1.59	0.67
1:E:424:PHE:HB2	1:E:527:THR:HG22	1.75	0.67
1:H:563:LEU:HB3	1:H:569:ILE:HG23	1.76	0.67
1:E:563:LEU:HB3	1:E:569:ILE:HG23	1.76	0.67
1:G:563:LEU:HB3	1:G:569:ILE:HG23	1.75	0.67
1:G:621:MET:HE3	2:7:46:ILE:HB	1.76	0.67
1:D:353:LEU:HD11	1:D:517:ARG:HH22	1.60	0.67
1:I:417:PRO:HG2	1:J:570:GLN:NE2	2.10	0.67
1:J:533:VAL:HG13	1:J:537:LEU:HD23	1.77	0.66
1:B:349:ARG:HH11	1:B:517:ARG:HD3	1.58	0.66
1:I:353:LEU:HD11	1:I:517:ARG:HH22	1.61	0.66
1:I:563:LEU:HB3	1:I:569:ILE:HG23	1.76	0.66
1:C:424:PHE:HB2	1:C:527:THR:HG22	1.75	0.66
1:C:559:ARG:HD2	1:C:623:ILE:HA	1.78	0.66
1:E:353:LEU:HD11	1:E:517:ARG:HH22	1.61	0.66
1:E:533:VAL:HG13	1:E:537:LEU:HD23	1.77	0.66
1:F:563:LEU:HB3	1:F:569:ILE:HG23	1.76	0.66
1:K:339:GLN:NE2	1:L:333:GLN:H	1.93	0.66
1:L:559:ARG:HD2	1:L:623:ILE:HA	1.78	0.66
1:A:353:LEU:HD11	1:A:517:ARG:HH22	1.61	0.66
1:B:353:LEU:HD11	1:B:517:ARG:HH22	1.61	0.66
1:D:559:ARG:HD2	1:D:623:ILE:HA	1.78	0.66
1:E:559:ARG:HD2	1:E:623:ILE:HA	1.77	0.66
1:D:533:VAL:HG13	1:D:537:LEU:HD23	1.77	0.66
1:D:563:LEU:HB3	1:D:569:ILE:HG23	1.76	0.65
1:K:533:VAL:HG13	1:K:537:LEU:HD23	1.78	0.65
1:A:533:VAL:HG13	1:A:537:LEU:HD23	1.78	0.65
1:B:563:LEU:HB3	1:B:569:ILE:HG23	1.77	0.65
1:H:533:VAL:HG13	1:H:537:LEU:HD23	1.78	0.65
1:I:448:LEU:HD21	1:I:463:VAL:HB	1.78	0.65
1:K:559:ARG:HD2	1:K:623:ILE:HA	1.78	0.65
1:F:353:LEU:HD11	1:F:517:ARG:HH22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:448:LEU:HD21	1:F:463:VAL:HB	1.79	0.65
1:F:559:ARG:HD2	1:F:623:ILE:HA	1.78	0.65
1:K:508:ASN:HD21	1:L:448:LEU:HD23	1.60	0.65
1:A:559:ARG:HD2	1:A:623:ILE:HA	1.78	0.65
1:I:343:THR:HG23	1:J:293:LEU:HD13	1.77	0.65
1:C:533:VAL:HG13	1:C:537:LEU:HD23	1.77	0.65
1:H:559:ARG:HD2	1:H:623:ILE:HA	1.77	0.65
1:H:353:LEU:HD11	1:H:517:ARG:HH22	1.61	0.65
1:J:559:ARG:HD2	1:J:623:ILE:HA	1.77	0.65
1:K:448:LEU:HD21	1:K:463:VAL:HB	1.79	0.65
1:J:353:LEU:HD11	1:J:517:ARG:HH22	1.61	0.65
1:C:353:LEU:HD11	1:C:517:ARG:HH22	1.60	0.64
1:G:353:LEU:HD11	1:G:517:ARG:HH22	1.61	0.64
1:L:533:VAL:HG13	1:L:537:LEU:HD23	1.77	0.64
1:B:448:LEU:HD21	1:B:463:VAL:HB	1.79	0.64
1:B:533:VAL:HG13	1:B:537:LEU:HD23	1.79	0.64
1:B:559:ARG:HD2	1:B:623:ILE:HA	1.78	0.64
1:F:396:CYS:HA	2:6:14:ILE:HG21	1.79	0.64
1:G:559:ARG:HD2	1:G:623:ILE:HA	1.77	0.64
1:A:448:LEU:HD21	1:A:463:VAL:HB	1.79	0.64
1:G:533:VAL:HG13	1:G:537:LEU:HD23	1.79	0.64
1:K:353:LEU:HD11	1:K:517:ARG:HH22	1.61	0.64
1:E:448:LEU:HD21	1:E:463:VAL:HB	1.79	0.64
1:L:284:ASP:HB3	1:L:287:LEU:HB3	1.80	0.64
1:G:448:LEU:HD21	1:G:463:VAL:HB	1.80	0.64
1:K:420:ARG:HB3	1:K:523:PRO:HB3	1.80	0.64
1:C:448:LEU:HD21	1:C:463:VAL:HB	1.79	0.64
1:H:284:ASP:HB3	1:H:287:LEU:HB3	1.80	0.64
1:I:559:ARG:HD2	1:I:623:ILE:HA	1.78	0.64
1:B:420:ARG:HB3	1:B:523:PRO:HB3	1.80	0.64
1:G:284:ASP:HB3	1:G:287:LEU:HB3	1.79	0.64
1:J:420:ARG:HB3	1:J:523:PRO:HB3	1.80	0.64
1:D:448:LEU:HD21	1:D:463:VAL:HB	1.79	0.64
1:L:353:LEU:HD11	1:L:517:ARG:HH22	1.62	0.64
1:A:620:ALA:HB2	2:1:15:PHE:CZ	2.34	0.63
1:B:332:ASN:HB3	1:B:335:THR:HB	1.80	0.63
1:I:533:VAL:HG13	1:I:537:LEU:HD23	1.80	0.63
1:J:448:LEU:HD21	1:J:463:VAL:HB	1.79	0.63
1:K:332:ASN:HB3	1:K:335:THR:HB	1.80	0.63
1:E:284:ASP:HB3	1:E:287:LEU:HB3	1.79	0.63
1:H:448:LEU:HD21	1:H:463:VAL:HB	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:284:ASP:HB3	1:I:287:LEU:HB3	1.80	0.63
1:J:339:GLN:HE21	1:K:333:GLN:H	1.46	0.63
1:C:284:ASP:HB3	1:C:287:LEU:HB3	1.80	0.63
1:F:284:ASP:HB3	1:F:287:LEU:HB3	1.79	0.63
1:J:284:ASP:HB3	1:J:287:LEU:HB3	1.79	0.63
1:L:448:LEU:HD21	1:L:463:VAL:HB	1.79	0.63
1:F:420:ARG:HB3	1:F:523:PRO:HB3	1.81	0.63
1:F:533:VAL:HG13	1:F:537:LEU:HD23	1.80	0.63
1:A:420:ARG:HB3	1:A:523:PRO:HB3	1.80	0.63
1:B:284:ASP:HB3	1:B:287:LEU:HB3	1.79	0.63
1:D:535:LYS:HE2	1:E:484:ASP:HB2	1.81	0.63
1:D:332:ASN:HB3	1:D:335:THR:HB	1.81	0.63
1:I:420:ARG:HB3	1:I:523:PRO:HB3	1.80	0.63
1:L:420:ARG:HB3	1:L:523:PRO:HB3	1.80	0.63
1:E:420:ARG:HB3	1:E:523:PRO:HB3	1.80	0.63
1:H:332:ASN:HB3	1:H:335:THR:HB	1.81	0.63
1:E:332:ASN:HB3	1:E:335:THR:HB	1.81	0.63
1:K:284:ASP:HB3	1:K:287:LEU:HB3	1.79	0.63
1:G:620:ALA:HB2	2:7:15:PHE:CZ	2.34	0.62
1:D:284:ASP:HB3	1:D:287:LEU:HB3	1.80	0.62
1:E:548:ARG:HH12	2:5:10:GLU:HG3	1.65	0.62
1:F:332:ASN:HB3	1:F:335:THR:HB	1.81	0.62
1:J:332:ASN:HB3	1:J:335:THR:HB	1.80	0.62
1:B:618:ASN:HB3	1:B:623:ILE:HG13	1.81	0.62
1:F:618:ASN:HB3	1:F:623:ILE:HG13	1.81	0.62
1:H:618:ASN:HB3	1:H:623:ILE:HG13	1.81	0.62
1:D:420:ARG:HB3	1:D:523:PRO:HB3	1.80	0.62
1:L:332:ASN:HB3	1:L:335:THR:HB	1.81	0.62
1:A:284:ASP:HB3	1:A:287:LEU:HB3	1.80	0.62
1:G:420:ARG:HB3	1:G:523:PRO:HB3	1.80	0.62
1:G:618:ASN:HB3	1:G:623:ILE:HG13	1.81	0.62
1:G:332:ASN:HB3	1:G:335:THR:HB	1.80	0.62
1:C:618:ASN:HB3	1:C:623:ILE:HG13	1.81	0.62
1:D:618:ASN:HB3	1:D:623:ILE:HG13	1.81	0.62
1:C:332:ASN:HB3	1:C:335:THR:HB	1.81	0.62
1:I:618:ASN:HB3	1:I:623:ILE:HG13	1.81	0.62
1:K:618:ASN:HB3	1:K:623:ILE:HG13	1.81	0.62
1:L:618:ASN:HB3	1:L:623:ILE:HG13	1.82	0.62
1:B:472:PHE:HD2	1:B:526:VAL:HG22	1.65	0.61
1:C:420:ARG:HB3	1:C:523:PRO:HB3	1.80	0.61
1:G:472:PHE:HD2	1:G:526:VAL:HG22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:420:ARG:HB3	1:H:523:PRO:HB3	1.80	0.61
1:K:472:PHE:HD2	1:K:526:VAL:HG22	1.66	0.61
1:E:349:ARG:HH12	1:E:517:ARG:HB2	1.65	0.61
1:H:349:ARG:HH12	1:H:517:ARG:HB2	1.66	0.61
1:K:349:ARG:HH12	1:K:517:ARG:HB2	1.66	0.61
1:A:333:GLN:H	1:F:339:GLN:NE2	1.99	0.61
1:A:349:ARG:HH12	1:A:517:ARG:HB2	1.66	0.61
1:I:332:ASN:HB3	1:I:335:THR:HB	1.82	0.61
1:C:472:PHE:HD2	1:C:526:VAL:HG22	1.66	0.61
1:D:349:ARG:HH12	1:D:517:ARG:HB2	1.66	0.61
1:I:349:ARG:HH12	1:I:517:ARG:HB2	1.66	0.61
1:J:618:ASN:HB3	1:J:623:ILE:HG13	1.82	0.61
1:A:332:ASN:HB3	1:A:335:THR:HB	1.81	0.60
1:A:618:ASN:HB3	1:A:623:ILE:HG13	1.82	0.60
1:E:472:PHE:HD2	1:E:526:VAL:HG22	1.66	0.60
1:E:618:ASN:HB3	1:E:623:ILE:HG13	1.82	0.60
1:D:472:PHE:HD2	1:D:526:VAL:HG22	1.66	0.60
1:C:514:LEU:HD23	1:C:514:LEU:H	1.67	0.60
1:F:472:PHE:HD2	1:F:526:VAL:HG22	1.66	0.60
1:J:349:ARG:HH12	1:J:517:ARG:HB2	1.66	0.60
1:J:472:PHE:HD2	1:J:526:VAL:HG22	1.66	0.60
1:L:349:ARG:HH12	1:L:517:ARG:HB2	1.66	0.60
1:H:472:PHE:HD2	1:H:526:VAL:HG22	1.66	0.60
1:A:472:PHE:HD2	1:A:526:VAL:HG22	1.66	0.59
1:C:349:ARG:HH12	1:C:517:ARG:HB2	1.66	0.59
1:E:417:PRO:HG2	1:F:570:GLN:NE2	2.16	0.59
1:G:349:ARG:HH12	1:G:517:ARG:HB2	1.67	0.59
1:I:472:PHE:HD2	1:I:526:VAL:HG22	1.67	0.59
1:L:472:PHE:HD2	1:L:526:VAL:HG22	1.66	0.59
1:D:514:LEU:H	1:D:514:LEU:HD23	1.67	0.59
1:L:514:LEU:HD23	1:L:514:LEU:H	1.67	0.59
1:A:514:LEU:HD23	1:A:514:LEU:H	1.67	0.59
1:A:621:MET:HE1	2:1:46:ILE:HB	1.85	0.59
1:K:339:GLN:HE21	1:L:333:GLN:H	1.51	0.59
1:K:417:PRO:HG2	1:L:570:GLN:HE21	1.67	0.59
1:A:337:CYS:O	1:A:341:VAL:HG23	2.03	0.59
1:B:514:LEU:HD23	1:B:514:LEU:H	1.68	0.59
1:F:349:ARG:HH12	1:F:517:ARG:HB2	1.66	0.59
2:2:30:LEU:HD21	2:2:66:GLU:HG2	1.84	0.59
2:U:30:LEU:HD21	2:U:66:GLU:HG2	1.84	0.59
2:7:30:LEU:HD21	2:7:66:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:30:LEU:HD21	2:8:66:GLU:HG2	1.85	0.59
1:G:514:LEU:HD23	1:G:514:LEU:H	1.68	0.59
1:H:337:CYS:O	1:H:341:VAL:HG23	2.03	0.59
2:3:30:LEU:HD21	2:3:66:GLU:HG2	1.85	0.59
2:1:30:LEU:HD21	2:1:66:GLU:HG2	1.84	0.59
2:4:30:LEU:HD21	2:4:66:GLU:HG2	1.84	0.59
1:B:349:ARG:HH12	1:B:517:ARG:HB2	1.66	0.59
1:I:514:LEU:H	1:I:514:LEU:HD23	1.68	0.59
2:W:30:LEU:HD21	2:W:66:GLU:HG2	1.84	0.59
2:U:17:LEU:HD22	2:U:57:LEU:HD11	1.84	0.58
1:K:337:CYS:O	1:K:341:VAL:HG23	2.03	0.58
1:L:337:CYS:O	1:L:341:VAL:HG23	2.03	0.58
1:D:337:CYS:O	1:D:341:VAL:HG23	2.03	0.58
1:D:339:GLN:HE21	1:E:333:GLN:H	1.48	0.58
2:9:30:LEU:HD21	2:9:66:GLU:HG2	1.84	0.58
1:G:337:CYS:O	1:G:341:VAL:HG23	2.03	0.58
1:I:337:CYS:O	1:I:341:VAL:HG23	2.03	0.58
1:K:514:LEU:H	1:K:514:LEU:HD23	1.67	0.58
2:U:54:LYS:HD3	2:U:61:ILE:HG12	1.85	0.58
2:5:30:LEU:HD21	2:5:66:GLU:HG2	1.84	0.58
1:A:293:LEU:HD13	1:F:343:THR:HG23	1.86	0.58
1:H:514:LEU:HD23	1:H:514:LEU:H	1.68	0.58
1:B:337:CYS:O	1:B:341:VAL:HG23	2.03	0.58
1:J:337:CYS:O	1:J:341:VAL:HG23	2.03	0.58
2:W:17:LEU:HD22	2:W:57:LEU:HD11	1.86	0.58
1:D:548:ARG:CZ	2:4:10:GLU:HG3	2.34	0.58
1:A:333:GLN:H	1:F:339:GLN:HE21	1.51	0.58
1:C:337:CYS:O	1:C:341:VAL:HG23	2.04	0.58
1:C:508:ASN:HD21	1:D:448:LEU:HD23	1.69	0.58
1:I:339:GLN:HE21	1:J:333:GLN:H	1.50	0.58
2:5:17:LEU:HD22	2:5:57:LEU:HD11	1.86	0.58
1:E:514:LEU:HD23	1:E:514:LEU:H	1.68	0.58
2:2:45:LEU:HD21	2:2:62:LEU:HD13	1.86	0.58
1:J:514:LEU:HD23	1:J:514:LEU:H	1.69	0.57
2:1:45:LEU:HD21	2:1:62:LEU:HD13	1.86	0.57
1:E:337:CYS:O	1:E:341:VAL:HG23	2.03	0.57
1:F:514:LEU:HD23	1:F:514:LEU:H	1.69	0.57
2:8:45:LEU:HD21	2:8:62:LEU:HD13	1.86	0.57
1:G:423:LEU:HD23	1:G:544:GLN:HG3	1.86	0.57
1:I:339:GLN:NE2	1:J:333:GLN:H	2.02	0.57
2:6:30:LEU:HD21	2:6:66:GLU:HG2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ASP:HB2	1:F:535:LYS:HE2	1.87	0.57
1:G:291:MET:SD	1:L:350:VAL:HG13	2.44	0.57
2:U:54:LYS:HD3	2:U:61:ILE:CD1	2.34	0.57
1:C:339:GLN:NE2	1:D:333:GLN:H	2.02	0.57
2:7:45:LEU:HD21	2:7:62:LEU:HD13	1.86	0.57
2:3:45:LEU:HD21	2:3:62:LEU:HD13	1.86	0.57
1:F:337:CYS:O	1:F:341:VAL:HG23	2.03	0.57
2:7:17:LEU:HD22	2:7:57:LEU:HD11	1.87	0.57
2:1:17:LEU:HD22	2:1:57:LEU:HD11	1.87	0.57
1:B:548:ARG:CZ	2:2:7:GLN:HE21	2.17	0.57
1:H:465:ILE:HG12	1:H:509:LEU:HD13	1.87	0.57
1:I:465:ILE:HG12	1:I:509:LEU:HD13	1.87	0.57
2:6:45:LEU:HD21	2:6:62:LEU:HD13	1.87	0.57
2:4:45:LEU:HD21	2:4:62:LEU:HD13	1.87	0.57
1:H:423:LEU:HD23	1:H:544:GLN:HG3	1.87	0.56
2:3:17:LEU:HD22	2:3:57:LEU:HD11	1.87	0.56
2:9:45:LEU:HD21	2:9:62:LEU:HD13	1.87	0.56
2:5:45:LEU:HD21	2:5:62:LEU:HD13	1.86	0.56
1:E:423:LEU:HD23	1:E:544:GLN:HG3	1.87	0.56
1:I:517:ARG:HH12	1:J:287:LEU:HD22	1.70	0.56
2:4:11:GLU:HA	2:4:14:ILE:HD12	1.86	0.56
1:A:465:ILE:HG12	1:A:509:LEU:HD13	1.88	0.56
1:D:465:ILE:HG12	1:D:509:LEU:HD13	1.88	0.56
1:L:423:LEU:HD23	1:L:544:GLN:HG3	1.88	0.56
1:B:423:LEU:HD23	1:B:544:GLN:HG3	1.88	0.56
1:C:465:ILE:HG12	1:C:509:LEU:HD13	1.88	0.56
1:D:423:LEU:HD23	1:D:544:GLN:HG3	1.86	0.56
1:E:613:GLN:HE21	1:E:613:GLN:H	1.54	0.56
1:I:423:LEU:HD23	1:I:544:GLN:HG3	1.87	0.56
2:8:17:LEU:HD22	2:8:57:LEU:HD11	1.88	0.56
2:9:17:LEU:HD22	2:9:57:LEU:HD11	1.88	0.56
1:E:499:ASP:HB3	1:F:473:GLU:HG3	1.88	0.56
1:D:343:THR:HG23	1:E:293:LEU:HD13	1.86	0.56
1:J:465:ILE:HG12	1:J:509:LEU:HD13	1.88	0.56
1:D:613:GLN:H	1:D:613:GLN:HE21	1.53	0.56
1:J:343:THR:HG23	1:K:293:LEU:HD13	1.87	0.56
2:6:17:LEU:HD22	2:6:57:LEU:HD11	1.87	0.56
2:U:45:LEU:HD21	2:U:62:LEU:HD13	1.87	0.56
2:W:45:LEU:HD21	2:W:62:LEU:HD13	1.86	0.56
1:B:548:ARG:NH1	2:2:7:GLN:HE21	2.04	0.55
1:G:567:ARG:HE	1:L:417:PRO:HD3	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:423:LEU:HD23	1:K:544:GLN:HG3	1.88	0.55
1:B:465:ILE:HG12	1:B:509:LEU:HD13	1.88	0.55
1:J:613:GLN:HE21	1:J:613:GLN:H	1.54	0.55
1:G:465:ILE:HG12	1:G:509:LEU:HD13	1.88	0.55
1:I:266:LYS:HE3	1:I:266:LYS:HA	1.87	0.55
2:4:17:LEU:HD22	2:4:57:LEU:HD11	1.87	0.55
1:E:465:ILE:HG12	1:E:509:LEU:HD13	1.87	0.55
1:J:497:LEU:HB3	1:J:500:TYR:HB2	1.88	0.55
1:K:497:LEU:HB3	1:K:500:TYR:HB2	1.89	0.55
1:B:613:GLN:H	1:B:613:GLN:HE21	1.53	0.55
1:L:552:TYR:CD2	2:W:39:GLU:HB3	2.41	0.55
1:F:613:GLN:H	1:F:613:GLN:HE21	1.54	0.55
1:C:349:ARG:HH21	1:D:286:LEU:HD12	1.70	0.55
1:K:465:ILE:HG12	1:K:509:LEU:HD13	1.87	0.55
2:2:17:LEU:HD22	2:2:57:LEU:HD11	1.87	0.55
2:8:11:GLU:HA	2:8:14:ILE:HD12	1.89	0.55
1:C:497:LEU:HB3	1:C:500:TYR:HB2	1.89	0.55
1:D:497:LEU:HB3	1:D:500:TYR:HB2	1.89	0.55
1:G:497:LEU:HB3	1:G:500:TYR:HB2	1.89	0.55
1:H:497:LEU:HB3	1:H:500:TYR:HB2	1.89	0.55
1:A:423:LEU:HD23	1:A:544:GLN:HG3	1.89	0.55
1:J:423:LEU:HD23	1:J:544:GLN:HG3	1.88	0.55
1:L:497:LEU:HB3	1:L:500:TYR:HB2	1.89	0.55
1:C:423:LEU:HD23	1:C:544:GLN:HG3	1.88	0.55
1:F:423:LEU:HD23	1:F:544:GLN:HG3	1.88	0.55
1:E:497:LEU:HB3	1:E:500:TYR:HB2	1.89	0.54
1:F:497:LEU:HB3	1:F:500:TYR:HB2	1.89	0.54
1:H:613:GLN:H	1:H:613:GLN:HE21	1.56	0.54
1:J:589:ALA:O	1:J:593:GLN:HG3	2.08	0.54
1:F:465:ILE:HG12	1:F:509:LEU:HD13	1.88	0.54
1:G:331:LYS:C	1:L:339:GLN:HE22	2.10	0.54
1:A:613:GLN:H	1:A:613:GLN:HE21	1.56	0.54
1:C:372:MET:HA	1:C:375:MET:HG2	1.90	0.54
1:C:589:ALA:O	1:C:593:GLN:HG3	2.08	0.54
1:I:497:LEU:HB3	1:I:500:TYR:HB2	1.88	0.54
1:A:497:LEU:HB3	1:A:500:TYR:HB2	1.89	0.54
1:H:372:MET:HA	1:H:375:MET:HG2	1.90	0.54
1:B:372:MET:HA	1:B:375:MET:HG2	1.90	0.54
1:B:417:PRO:HG2	1:C:570:GLN:HE21	1.73	0.54
1:D:401:MET:O	1:D:405:VAL:HG23	2.08	0.54
1:L:589:ALA:O	1:L:593:GLN:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:GLN:H	1:L:339:GLN:NE2	2.05	0.54
1:I:613:GLN:H	1:I:613:GLN:HE21	1.55	0.54
1:J:372:MET:HA	1:J:375:MET:HG2	1.90	0.54
1:K:372:MET:HA	1:K:375:MET:HG2	1.90	0.54
1:L:465:ILE:HG12	1:L:509:LEU:HD13	1.88	0.54
1:G:613:GLN:H	1:G:613:GLN:HE21	1.55	0.54
1:A:589:ALA:O	1:A:593:GLN:HG3	2.07	0.54
1:B:497:LEU:HB3	1:B:500:TYR:HB2	1.89	0.54
1:B:581:TRP:HE3	1:B:603:LEU:HD23	1.73	0.54
1:E:589:ALA:O	1:E:593:GLN:HG3	2.08	0.54
1:H:550:LYS:HD3	1:H:552:TYR:OH	2.08	0.54
2:3:11:GLU:HA	2:3:14:ILE:HD12	1.91	0.53
1:H:581:TRP:HE3	1:H:603:LEU:HD23	1.74	0.53
1:J:340:ALA:O	1:J:344:VAL:HG23	2.08	0.53
1:K:613:GLN:H	1:K:613:GLN:HE21	1.55	0.53
2:6:11:GLU:HA	2:6:14:ILE:HD12	1.90	0.53
1:B:589:ALA:O	1:B:593:GLN:HG3	2.08	0.53
1:I:340:ALA:O	1:I:344:VAL:HG23	2.08	0.53
2:2:11:GLU:HA	2:2:14:ILE:HD12	1.91	0.53
1:B:340:ALA:O	1:B:344:VAL:HG23	2.08	0.53
1:C:504:SER:HB2	1:D:433:THR:HG22	1.91	0.53
1:F:340:ALA:O	1:F:344:VAL:HG23	2.08	0.53
1:F:401:MET:O	1:F:405:VAL:HG23	2.09	0.53
1:G:401:MET:O	1:G:405:VAL:HG23	2.09	0.53
2:U:11:GLU:HB3	2:U:42:VAL:HG11	1.91	0.53
1:E:401:MET:O	1:E:405:VAL:HG23	2.08	0.53
1:H:340:ALA:O	1:H:344:VAL:HG23	2.08	0.53
1:I:581:TRP:HE3	1:I:603:LEU:HD23	1.73	0.53
1:J:349:ARG:NH1	1:J:517:ARG:HD3	2.23	0.53
1:L:581:TRP:HE3	1:L:603:LEU:HD23	1.74	0.53
1:L:613:GLN:H	1:L:613:GLN:HE21	1.55	0.53
1:A:340:ALA:O	1:A:344:VAL:HG23	2.09	0.53
1:E:372:MET:HA	1:E:375:MET:HG2	1.90	0.53
1:C:581:TRP:HE3	1:C:603:LEU:HD23	1.74	0.53
1:D:581:TRP:HE3	1:D:603:LEU:HD23	1.73	0.53
1:E:340:ALA:O	1:E:344:VAL:HG23	2.08	0.53
1:F:349:ARG:NH1	1:F:517:ARG:HD3	2.24	0.53
1:G:340:ALA:O	1:G:344:VAL:HG23	2.08	0.53
1:G:372:MET:HA	1:G:375:MET:HG2	1.90	0.53
1:H:339:GLN:NE2	1:I:333:GLN:H	2.07	0.53
1:K:343:THR:HG23	1:L:293:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:303:LEU:HD23	1:L:307:LYS:HZ1	1.74	0.53
2:2:11:GLU:HB3	2:2:42:VAL:HG11	1.91	0.53
1:D:372:MET:HA	1:D:375:MET:HG2	1.90	0.53
1:E:581:TRP:HE3	1:E:603:LEU:HD23	1.74	0.53
1:F:581:TRP:HE3	1:F:603:LEU:HD23	1.74	0.53
1:G:581:TRP:HE3	1:G:603:LEU:HD23	1.74	0.53
1:I:372:MET:HA	1:I:375:MET:HG2	1.90	0.53
1:H:589:ALA:O	1:H:593:GLN:HG3	2.08	0.53
1:K:349:ARG:NH1	1:K:517:ARG:HD3	2.24	0.53
1:K:589:ALA:O	1:K:593:GLN:HG3	2.09	0.53
2:9:11:GLU:HB3	2:9:42:VAL:HG11	1.91	0.53
1:A:581:TRP:HE3	1:A:603:LEU:HD23	1.74	0.52
1:D:340:ALA:O	1:D:344:VAL:HG23	2.09	0.52
1:E:349:ARG:NH1	1:E:517:ARG:HD3	2.23	0.52
1:I:349:ARG:NH1	1:I:517:ARG:HD3	2.23	0.52
1:I:589:ALA:O	1:I:593:GLN:HG3	2.08	0.52
1:J:388:MET:HE3	1:J:577:LEU:HD13	1.91	0.52
2:5:11:GLU:HB3	2:5:42:VAL:HG11	1.91	0.52
1:C:613:GLN:H	1:C:613:GLN:HE21	1.55	0.52
1:F:372:MET:HA	1:F:375:MET:HG2	1.90	0.52
1:J:581:TRP:HE3	1:J:603:LEU:HD23	1.73	0.52
2:6:11:GLU:HB3	2:6:42:VAL:HG11	1.91	0.52
2:6:74:LEU:HD13	2:6:77:ALA:HB3	1.91	0.52
1:A:508:ASN:HD21	1:B:448:LEU:HD23	1.73	0.52
1:C:340:ALA:O	1:C:344:VAL:HG23	2.09	0.52
1:C:401:MET:O	1:C:405:VAL:HG23	2.10	0.52
1:F:589:ALA:O	1:F:593:GLN:HG3	2.08	0.52
1:K:581:TRP:HE3	1:K:603:LEU:HD23	1.74	0.52
1:L:372:MET:HA	1:L:375:MET:HG2	1.90	0.52
1:C:349:ARG:NH1	1:C:517:ARG:HD3	2.23	0.52
1:I:621:MET:SD	2:9:47:ALA:HB2	2.49	0.52
2:5:11:GLU:HA	2:5:14:ILE:HD12	1.91	0.52
2:7:11:GLU:HB3	2:7:42:VAL:HG11	1.91	0.52
1:A:372:MET:HA	1:A:375:MET:HG2	1.90	0.52
1:J:550:LYS:HD3	1:J:552:TYR:OH	2.09	0.52
1:D:589:ALA:O	1:D:593:GLN:HG3	2.09	0.52
1:G:286:LEU:HD12	1:L:349:ARG:NH2	2.02	0.52
1:G:589:ALA:O	1:G:593:GLN:HG3	2.09	0.52
1:I:401:MET:O	1:I:405:VAL:HG23	2.10	0.52
1:J:401:MET:O	1:J:405:VAL:HG23	2.10	0.52
1:L:401:MET:O	1:L:405:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:11:GLU:HB3	2:W:42:VAL:HG11	1.92	0.52
2:3:11:GLU:HB3	2:3:42:VAL:HG11	1.91	0.52
2:6:11:GLU:HB2	2:6:42:VAL:HG21	1.92	0.52
2:9:11:GLU:HA	2:9:14:ILE:HD12	1.91	0.52
1:C:621:MET:SD	2:3:47:ALA:HB2	2.50	0.52
1:K:340:ALA:O	1:K:344:VAL:HG23	2.09	0.52
2:U:11:GLU:HB2	2:U:42:VAL:HG21	1.92	0.52
2:4:11:GLU:HB2	2:4:42:VAL:HG21	1.92	0.52
1:A:401:MET:O	1:A:405:VAL:HG23	2.10	0.52
1:B:349:ARG:NH1	1:B:517:ARG:HD3	2.24	0.52
1:B:401:MET:O	1:B:405:VAL:HG23	2.10	0.52
1:B:548:ARG:NH2	2:2:7:GLN:HE21	2.08	0.52
1:J:508:ASN:HD21	1:K:448:LEU:HD23	1.74	0.52
1:L:340:ALA:O	1:L:344:VAL:HG23	2.08	0.52
2:1:11:GLU:HB3	2:1:42:VAL:HG11	1.92	0.52
1:A:349:ARG:NH1	1:A:517:ARG:HD3	2.24	0.51
1:C:388:MET:HE3	1:C:577:LEU:HD13	1.93	0.51
1:E:417:PRO:HD3	1:F:567:ARG:HE	1.74	0.51
1:F:349:ARG:NH1	1:F:517:ARG:HB2	2.25	0.51
1:H:349:ARG:NH1	1:H:517:ARG:HB2	2.25	0.51
1:H:349:ARG:NH1	1:H:517:ARG:HD3	2.24	0.51
1:I:388:MET:HE3	1:I:577:LEU:HD13	1.92	0.51
2:W:11:GLU:HA	2:W:14:ILE:HD12	1.91	0.51
2:7:11:GLU:HA	2:7:14:ILE:HD12	1.91	0.51
2:7:11:GLU:HB2	2:7:42:VAL:HG21	1.92	0.51
2:9:11:GLU:HB2	2:9:42:VAL:HG21	1.92	0.51
1:A:550:LYS:HD3	1:A:552:TYR:OH	2.11	0.51
2:5:11:GLU:HB2	2:5:42:VAL:HG21	1.93	0.51
1:C:417:PRO:HG2	1:D:570:GLN:NE2	2.23	0.51
1:J:349:ARG:NH1	1:J:517:ARG:HB2	2.25	0.51
2:U:74:LEU:HD13	2:U:77:ALA:HB3	1.92	0.51
2:8:11:GLU:HB2	2:8:42:VAL:HG21	1.93	0.51
2:8:11:GLU:HB3	2:8:42:VAL:HG11	1.92	0.51
1:G:448:LEU:HD23	1:L:508:ASN:HD21	1.74	0.51
2:5:74:LEU:HD13	2:5:77:ALA:HB3	1.92	0.51
2:7:74:LEU:HD13	2:7:77:ALA:HB3	1.92	0.51
2:1:11:GLU:HB2	2:1:42:VAL:HG21	1.93	0.51
1:B:550:LYS:HD3	1:B:552:TYR:OH	2.11	0.51
1:D:388:MET:HE3	1:D:577:LEU:HD13	1.93	0.51
1:L:349:ARG:NH1	1:L:517:ARG:HB2	2.25	0.51
2:W:74:LEU:HD13	2:W:77:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:74:LEU:HD13	2:9:77:ALA:HB3	1.92	0.51
2:8:74:LEU:HD13	2:8:77:ALA:HB3	1.92	0.51
1:C:349:ARG:NH1	1:C:517:ARG:HB2	2.25	0.51
1:H:401:MET:O	1:H:405:VAL:HG23	2.10	0.51
1:K:401:MET:O	1:K:405:VAL:HG23	2.09	0.51
2:3:11:GLU:HB2	2:3:42:VAL:HG21	1.92	0.51
1:E:388:MET:HE3	1:E:577:LEU:HD13	1.93	0.51
1:E:550:LYS:HD3	1:E:552:TYR:OH	2.11	0.51
1:G:346:ALA:O	1:G:350:VAL:HG23	2.11	0.51
1:J:415:ASN:ND2	1:J:420:ARG:HD3	2.26	0.51
1:D:349:ARG:NH1	1:D:517:ARG:HD3	2.23	0.51
1:E:349:ARG:NH1	1:E:517:ARG:HB2	2.25	0.51
1:F:346:ALA:O	1:F:350:VAL:HG23	2.11	0.51
2:2:74:LEU:HD13	2:2:77:ALA:HB3	1.92	0.51
1:B:346:ALA:O	1:B:350:VAL:HG23	2.11	0.51
1:G:550:LYS:HD3	1:G:552:TYR:OH	2.10	0.51
1:I:349:ARG:NH1	1:I:517:ARG:HB2	2.26	0.51
2:3:74:LEU:HD13	2:3:77:ALA:HB3	1.93	0.51
2:U:11:GLU:HA	2:U:14:ILE:HD12	1.93	0.51
2:4:74:LEU:HD13	2:4:77:ALA:HB3	1.92	0.51
2:1:11:GLU:HA	2:1:14:ILE:HD12	1.92	0.51
2:1:74:LEU:HD13	2:1:77:ALA:HB3	1.93	0.51
1:B:349:ARG:NH1	1:B:517:ARG:HB2	2.26	0.50
1:B:388:MET:HE3	1:B:577:LEU:HD13	1.92	0.50
1:C:343:THR:HG23	1:D:293:LEU:HD13	1.92	0.50
1:F:396:CYS:HA	2:6:14:ILE:HG23	1.93	0.50
1:H:346:ALA:O	1:H:350:VAL:HG23	2.11	0.50
1:I:346:ALA:O	1:I:350:VAL:HG23	2.11	0.50
1:K:349:ARG:NH1	1:K:517:ARG:HB2	2.25	0.50
1:A:417:PRO:HG2	1:B:570:GLN:HE21	1.76	0.50
1:C:346:ALA:O	1:C:350:VAL:HG23	2.11	0.50
1:D:349:ARG:NH1	1:D:517:ARG:HB2	2.25	0.50
1:D:548:ARG:NH2	2:4:10:GLU:HG3	2.26	0.50
1:D:550:LYS:HD3	1:D:552:TYR:OH	2.11	0.50
1:E:346:ALA:O	1:E:350:VAL:HG23	2.11	0.50
1:F:550:LYS:HD3	1:F:552:TYR:OH	2.11	0.50
1:I:415:ASN:ND2	1:I:420:ARG:HD3	2.26	0.50
2:4:11:GLU:HB3	2:4:42:VAL:HG11	1.91	0.50
1:C:339:GLN:HE21	1:D:333:GLN:H	1.58	0.50
1:C:550:LYS:HD3	1:C:552:TYR:OH	2.11	0.50
1:K:346:ALA:O	1:K:350:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:415:ASN:ND2	1:K:420:ARG:HD3	2.26	0.50
1:G:388:MET:HE3	1:G:577:LEU:HD13	1.93	0.50
1:G:420:ARG:HD2	1:G:523:PRO:HB3	1.94	0.50
1:E:621:MET:SD	2:5:47:ALA:HB2	2.51	0.50
1:I:550:LYS:HD3	1:I:552:TYR:OH	2.11	0.50
1:A:415:ASN:ND2	1:A:420:ARG:HD3	2.27	0.50
1:C:415:ASN:ND2	1:C:420:ARG:HD3	2.27	0.50
1:E:415:ASN:ND2	1:E:420:ARG:HD3	2.26	0.50
1:G:349:ARG:NH1	1:G:517:ARG:HD3	2.25	0.50
1:K:517:ARG:HH12	1:L:287:LEU:HD22	1.75	0.50
1:A:349:ARG:NH1	1:A:517:ARG:HB2	2.25	0.50
1:L:550:LYS:HD3	1:L:552:TYR:OH	2.11	0.50
1:D:346:ALA:O	1:D:350:VAL:HG23	2.12	0.50
1:E:420:ARG:HD2	1:E:523:PRO:HB3	1.94	0.50
1:F:415:ASN:ND2	1:F:420:ARG:HD3	2.27	0.50
1:K:388:MET:HE3	1:K:577:LEU:HD13	1.94	0.50
1:L:388:MET:HE3	1:L:577:LEU:HD13	1.93	0.50
2:2:11:GLU:HB2	2:2:42:VAL:HG21	1.93	0.50
1:A:454:LEU:HG	1:A:493:ASN:ND2	2.27	0.49
1:K:550:LYS:HD3	1:K:552:TYR:OH	2.11	0.49
1:L:415:ASN:ND2	1:L:420:ARG:HD3	2.27	0.49
1:B:415:ASN:ND2	1:B:420:ARG:HD3	2.27	0.49
1:H:512:LYS:NZ	1:H:512:LYS:HB3	2.27	0.49
2:W:11:GLU:HB2	2:W:42:VAL:HG21	1.93	0.49
1:A:504:SER:HB2	1:B:433:THR:HG22	1.94	0.49
1:D:415:ASN:ND2	1:D:420:ARG:HD3	2.27	0.49
1:G:287:LEU:HD11	1:L:353:LEU:HD12	1.95	0.49
1:G:349:ARG:NH1	1:G:517:ARG:HB2	2.26	0.49
1:L:369:LEU:HD23	1:L:372:MET:SD	2.52	0.49
2:W:58:THR:O	2:W:62:LEU:HD23	2.13	0.49
1:G:415:ASN:ND2	1:G:420:ARG:HD3	2.26	0.49
1:H:454:LEU:HG	1:H:493:ASN:ND2	2.27	0.49
1:I:420:ARG:HD2	1:I:523:PRO:HB3	1.94	0.49
1:J:389:ALA:HB2	1:J:626:LEU:HD21	1.94	0.49
1:L:349:ARG:NH1	1:L:517:ARG:HD3	2.24	0.49
1:F:388:MET:HE3	1:F:577:LEU:HD13	1.93	0.49
1:J:450:VAL:HG23	1:J:490:GLY:HA2	1.94	0.49
1:L:420:ARG:HD2	1:L:523:PRO:HB3	1.95	0.49
2:9:58:THR:O	2:9:62:LEU:HD23	2.13	0.49
1:A:346:ALA:O	1:A:350:VAL:HG23	2.12	0.49
1:C:504:SER:O	1:D:437:ALA:HB1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:LEU:HD23	1:E:372:MET:SD	2.52	0.49
1:G:269:SER:HB3	1:G:272:LEU:HD12	1.95	0.49
2:U:54:LYS:HD3	2:U:61:ILE:CG1	2.43	0.49
1:H:415:ASN:ND2	1:H:420:ARG:HD3	2.27	0.49
1:K:454:LEU:HG	1:K:493:ASN:ND2	2.28	0.49
1:L:303:LEU:HB3	1:L:307:LYS:HZ3	1.78	0.49
1:C:369:LEU:HD23	1:C:372:MET:SD	2.53	0.49
1:F:420:ARG:HD2	1:F:523:PRO:HB3	1.95	0.49
1:G:450:VAL:HG23	1:G:490:GLY:HA2	1.95	0.49
1:K:369:LEU:HD23	1:K:372:MET:SD	2.53	0.49
1:D:450:VAL:HG23	1:D:490:GLY:HA2	1.95	0.49
1:D:454:LEU:HG	1:D:493:ASN:ND2	2.28	0.49
1:F:400:LYS:O	1:F:404:VAL:HG23	2.13	0.49
1:H:369:LEU:HD23	1:H:372:MET:SD	2.52	0.49
1:A:388:MET:HE3	1:A:577:LEU:HD13	1.95	0.49
1:C:400:LYS:O	1:C:404:VAL:HG23	2.13	0.49
1:C:615:MET:O	1:C:619:VAL:HG23	2.13	0.49
1:D:369:LEU:HD23	1:D:372:MET:SD	2.53	0.49
1:F:454:LEU:HG	1:F:493:ASN:ND2	2.28	0.49
1:G:409:LEU:O	1:G:413:VAL:HG23	2.13	0.49
1:H:615:MET:O	1:H:619:VAL:HG23	2.13	0.49
1:I:334:LYS:O	1:I:338:GLN:HB2	2.13	0.49
1:I:369:LEU:HD23	1:I:372:MET:SD	2.53	0.49
1:J:615:MET:O	1:J:619:VAL:HG23	2.13	0.49
2:5:58:THR:O	2:5:62:LEU:HD23	2.13	0.49
1:A:369:LEU:HD23	1:A:372:MET:SD	2.52	0.48
1:B:420:ARG:HD2	1:B:523:PRO:HB3	1.94	0.48
1:B:450:VAL:HG23	1:B:490:GLY:HA2	1.95	0.48
1:B:615:MET:O	1:B:619:VAL:HG23	2.13	0.48
1:D:552:TYR:OH	2:4:14:ILE:HG21	2.13	0.48
1:F:269:SER:HB3	1:F:272:LEU:HD12	1.95	0.48
1:F:512:LYS:NZ	1:F:512:LYS:HB3	2.28	0.48
1:F:615:MET:O	1:F:619:VAL:HG23	2.13	0.48
1:I:454:LEU:HG	1:I:493:ASN:ND2	2.28	0.48
1:J:369:LEU:HD23	1:J:372:MET:SD	2.54	0.48
1:J:420:ARG:HD2	1:J:523:PRO:HB3	1.94	0.48
2:2:58:THR:O	2:2:62:LEU:HD23	2.13	0.48
1:B:266:LYS:HG3	1:B:267:GLN:N	2.27	0.48
1:D:420:ARG:HD2	1:D:523:PRO:HB3	1.95	0.48
1:D:615:MET:O	1:D:619:VAL:HG23	2.13	0.48
1:F:369:LEU:HD23	1:F:372:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:334:LYS:O	1:G:338:GLN:HB2	2.13	0.48
1:G:369:LEU:HD23	1:G:372:MET:SD	2.53	0.48
1:G:454:LEU:HG	1:G:493:ASN:ND2	2.28	0.48
1:H:388:MET:HE3	1:H:577:LEU:HD13	1.95	0.48
1:I:389:ALA:HB2	1:I:626:LEU:HD21	1.94	0.48
1:K:499:ASP:HB3	1:L:473:GLU:CB	2.43	0.48
2:8:58:THR:O	2:8:62:LEU:HD23	2.13	0.48
1:B:409:LEU:O	1:B:413:VAL:HG23	2.13	0.48
1:B:512:LYS:NZ	1:B:512:LYS:HB3	2.29	0.48
1:G:535:LYS:HE2	1:H:484:ASP:HB2	1.96	0.48
1:I:354:GLN:CG	1:J:310:GLN:HG3	2.42	0.48
1:E:349:ARG:NH2	1:F:286:LEU:HD12	2.19	0.48
1:H:334:LYS:O	1:H:338:GLN:HB2	2.13	0.48
1:H:420:ARG:HD2	1:H:523:PRO:HB3	1.94	0.48
1:I:269:SER:HB3	1:I:272:LEU:HD12	1.94	0.48
1:I:420:ARG:HB3	1:I:523:PRO:CB	2.43	0.48
1:J:346:ALA:O	1:J:350:VAL:HG23	2.13	0.48
1:K:450:VAL:HG23	1:K:490:GLY:HA2	1.95	0.48
2:7:58:THR:O	2:7:62:LEU:HD23	2.13	0.48
2:1:58:THR:O	2:1:62:LEU:HD23	2.13	0.48
1:C:269:SER:HB3	1:C:272:LEU:HD12	1.95	0.48
1:C:303:LEU:H	1:C:303:LEU:HD12	1.78	0.48
1:C:512:LYS:NZ	1:C:512:LYS:HB3	2.28	0.48
1:C:518:THR:HG21	1:D:446:LYS:HD2	1.95	0.48
1:E:512:LYS:NZ	1:E:512:LYS:HB3	2.29	0.48
1:J:394:LEU:HD21	1:J:569:ILE:O	2.14	0.48
1:L:409:LEU:O	1:L:413:VAL:HG23	2.14	0.48
1:B:303:LEU:HD12	1:B:303:LEU:H	1.78	0.48
1:B:369:LEU:HD23	1:B:372:MET:SD	2.54	0.48
1:C:420:ARG:HD2	1:C:523:PRO:HB3	1.95	0.48
1:D:409:LEU:O	1:D:413:VAL:HG23	2.14	0.48
1:E:389:ALA:HB2	1:E:626:LEU:HD21	1.94	0.48
1:I:615:MET:O	1:I:619:VAL:HG23	2.13	0.48
1:J:269:SER:HB3	1:J:272:LEU:HD12	1.96	0.48
1:K:334:LYS:O	1:K:338:GLN:HB2	2.14	0.48
1:D:420:ARG:HB3	1:D:523:PRO:CB	2.44	0.48
1:E:334:LYS:O	1:E:338:GLN:HB2	2.13	0.48
1:F:389:ALA:HB2	1:F:626:LEU:HD21	1.96	0.48
1:F:450:VAL:HG23	1:F:490:GLY:HA2	1.95	0.48
1:J:334:LYS:O	1:J:338:GLN:HB2	2.14	0.48
1:B:420:ARG:HB3	1:B:523:PRO:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:LYS:O	1:D:338:GLN:HB2	2.14	0.48
1:D:400:LYS:O	1:D:404:VAL:HG23	2.14	0.48
1:E:454:LEU:HG	1:E:493:ASN:ND2	2.29	0.48
1:F:387:TRP:O	1:F:391:VAL:HG23	2.14	0.48
1:H:394:LEU:HD21	1:H:569:ILE:O	2.14	0.48
1:L:334:LYS:O	1:L:338:GLN:HB2	2.13	0.48
2:U:58:THR:O	2:U:62:LEU:HD23	2.14	0.48
1:A:400:LYS:O	1:A:404:VAL:HG23	2.13	0.48
1:B:394:LEU:HD21	1:B:569:ILE:O	2.14	0.48
1:C:454:LEU:HG	1:C:493:ASN:ND2	2.28	0.48
1:G:394:LEU:HD21	1:G:569:ILE:O	2.14	0.48
1:K:420:ARG:HD2	1:K:523:PRO:HB3	1.94	0.48
1:L:394:LEU:HD21	1:L:569:ILE:O	2.14	0.48
1:L:450:VAL:HG23	1:L:490:GLY:HA2	1.95	0.48
1:E:354:GLN:HG2	1:F:310:GLN:HG3	1.95	0.48
1:F:334:LYS:O	1:F:338:GLN:HB2	2.13	0.48
1:F:409:LEU:O	1:F:413:VAL:HG23	2.13	0.48
1:H:389:ALA:HB2	1:H:626:LEU:HD21	1.95	0.48
1:H:420:ARG:HB3	1:H:523:PRO:CB	2.44	0.48
1:H:504:SER:HB2	1:I:433:THR:HG22	1.94	0.48
1:J:454:LEU:HG	1:J:493:ASN:ND2	2.29	0.48
1:A:269:SER:HB3	1:A:272:LEU:HD12	1.96	0.47
1:A:303:LEU:HD12	1:A:303:LEU:H	1.79	0.47
1:E:615:MET:O	1:E:619:VAL:HG23	2.13	0.47
1:G:448:LEU:CD2	1:L:508:ASN:HD21	2.27	0.47
1:I:400:LYS:O	1:I:404:VAL:HG23	2.14	0.47
1:J:512:LYS:HB3	1:J:512:LYS:NZ	2.28	0.47
1:K:400:LYS:O	1:K:404:VAL:HG23	2.13	0.47
1:K:420:ARG:HB3	1:K:523:PRO:CB	2.44	0.47
1:K:615:MET:O	1:K:619:VAL:HG23	2.13	0.47
1:C:389:ALA:HB2	1:C:626:LEU:HD21	1.96	0.47
1:D:389:ALA:HB2	1:D:626:LEU:HD21	1.95	0.47
1:H:450:VAL:HG23	1:H:490:GLY:HA2	1.94	0.47
1:I:394:LEU:HD21	1:I:569:ILE:O	2.13	0.47
2:3:58:THR:O	2:3:62:LEU:HD23	2.14	0.47
2:4:58:THR:O	2:4:62:LEU:HD23	2.14	0.47
1:A:394:LEU:HD21	1:A:569:ILE:O	2.14	0.47
1:B:400:LYS:O	1:B:404:VAL:HG23	2.14	0.47
1:C:334:LYS:O	1:C:338:GLN:HB2	2.14	0.47
1:E:400:LYS:O	1:E:404:VAL:HG23	2.15	0.47
1:F:621:MET:HE1	2:6:46:ILE:CG2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:349:ARG:HG2	1:J:287:LEU:HA	1.96	0.47
1:K:269:SER:HB3	1:K:272:LEU:HD12	1.96	0.47
1:L:615:MET:O	1:L:619:VAL:HG23	2.13	0.47
1:A:615:MET:O	1:A:619:VAL:HG23	2.14	0.47
1:C:409:LEU:O	1:C:413:VAL:HG23	2.15	0.47
1:E:394:LEU:HD21	1:E:569:ILE:O	2.14	0.47
1:H:269:SER:HB3	1:H:272:LEU:HD12	1.95	0.47
1:I:450:VAL:HG23	1:I:490:GLY:HA2	1.96	0.47
1:J:420:ARG:HB3	1:J:523:PRO:CB	2.44	0.47
1:L:303:LEU:HD12	1:L:303:LEU:H	1.79	0.47
1:A:512:LYS:NZ	1:A:512:LYS:HB3	2.29	0.47
1:B:454:LEU:HG	1:B:493:ASN:ND2	2.29	0.47
1:C:394:LEU:HD21	1:C:569:ILE:O	2.14	0.47
1:F:554:LYS:O	1:F:558:GLU:HG3	2.15	0.47
1:K:303:LEU:HD12	1:K:303:LEU:H	1.80	0.47
1:K:389:ALA:HB2	1:K:626:LEU:HD21	1.97	0.47
1:K:554:LYS:O	1:K:558:GLU:HG3	2.15	0.47
1:L:269:SER:HB3	1:L:272:LEU:HD12	1.96	0.47
1:A:334:LYS:O	1:A:338:GLN:HB2	2.14	0.47
1:A:420:ARG:HD2	1:A:523:PRO:HB3	1.95	0.47
1:A:450:VAL:HG23	1:A:490:GLY:HA2	1.95	0.47
1:C:450:VAL:HG23	1:C:490:GLY:HA2	1.96	0.47
1:G:615:MET:O	1:G:619:VAL:HG23	2.14	0.47
1:I:512:LYS:NZ	1:I:512:LYS:HB3	2.29	0.47
1:J:535:LYS:HE2	1:K:484:ASP:HB2	1.96	0.47
1:K:512:LYS:NZ	1:K:512:LYS:HB3	2.29	0.47
1:L:389:ALA:HB2	1:L:626:LEU:HD21	1.96	0.47
2:6:58:THR:O	2:6:62:LEU:HD23	2.15	0.47
1:B:387:TRP:O	1:B:391:VAL:HG23	2.15	0.47
1:B:389:ALA:HB2	1:B:626:LEU:HD21	1.96	0.47
1:C:420:ARG:HB3	1:C:523:PRO:CB	2.44	0.47
1:D:269:SER:HB3	1:D:272:LEU:HD12	1.97	0.47
1:D:512:LYS:NZ	1:D:512:LYS:HB3	2.29	0.47
1:E:554:LYS:O	1:E:558:GLU:HG3	2.15	0.47
1:F:303:LEU:HD12	1:F:303:LEU:H	1.79	0.47
1:F:394:LEU:HD21	1:F:569:ILE:O	2.14	0.47
1:G:287:LEU:N	1:L:349:ARG:HG2	2.29	0.47
1:G:400:LYS:O	1:G:404:VAL:HG23	2.14	0.47
1:G:512:LYS:NZ	1:G:512:LYS:HB3	2.30	0.47
1:J:409:LEU:O	1:J:413:VAL:HG23	2.14	0.47
1:K:387:TRP:O	1:K:391:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:LYS:O	1:D:558:GLU:HG3	2.15	0.47
1:E:303:LEU:H	1:E:303:LEU:HD12	1.79	0.47
1:H:400:LYS:O	1:H:404:VAL:HG23	2.15	0.47
1:I:303:LEU:HD12	1:I:303:LEU:H	1.80	0.47
1:K:394:LEU:HD21	1:K:569:ILE:O	2.14	0.47
1:L:400:LYS:O	1:L:404:VAL:HG23	2.14	0.47
1:A:554:LYS:O	1:A:558:GLU:HG3	2.15	0.47
1:D:387:TRP:O	1:D:391:VAL:HG23	2.14	0.47
1:E:420:ARG:HB3	1:E:523:PRO:CB	2.44	0.47
1:G:554:LYS:O	1:G:558:GLU:HG3	2.15	0.47
1:L:454:LEU:HG	1:L:493:ASN:ND2	2.29	0.47
1:L:550:LYS:HB2	1:L:553:LEU:HD12	1.97	0.47
1:B:334:LYS:O	1:B:338:GLN:HB2	2.14	0.47
1:C:416:ILE:HG23	1:D:564:LEU:HB3	1.97	0.47
1:C:554:LYS:O	1:C:558:GLU:HG3	2.15	0.47
1:G:389:ALA:HB2	1:G:626:LEU:HD21	1.96	0.47
1:L:512:LYS:NZ	1:L:512:LYS:HB3	2.29	0.47
2:1:74:LEU:HD23	2:1:76:LYS:H	1.80	0.47
1:B:269:SER:HB3	1:B:272:LEU:HD12	1.97	0.46
1:B:554:LYS:O	1:B:558:GLU:HG3	2.15	0.46
1:E:269:SER:HB3	1:E:272:LEU:HD12	1.96	0.46
1:E:450:VAL:HG23	1:E:490:GLY:HA2	1.95	0.46
1:G:387:TRP:O	1:G:391:VAL:HG23	2.15	0.46
1:G:453:PRO:C	1:G:455:ASP:H	2.19	0.46
1:I:387:TRP:O	1:I:391:VAL:HG23	2.15	0.46
1:I:554:LYS:O	1:I:558:GLU:HG3	2.15	0.46
1:K:583:ARG:HA	1:K:584:PRO:HD3	1.83	0.46
1:B:504:SER:HB2	1:C:433:THR:HG22	1.96	0.46
1:C:439:LEU:HD23	1:C:575:LEU:HD13	1.97	0.46
1:E:387:TRP:O	1:E:391:VAL:HG23	2.15	0.46
1:E:590:GLN:HA	1:E:593:GLN:NE2	2.31	0.46
1:F:420:ARG:HB3	1:F:523:PRO:CB	2.45	0.46
1:J:387:TRP:O	1:J:391:VAL:HG23	2.15	0.46
2:8:74:LEU:HD23	2:8:76:LYS:H	1.80	0.46
1:B:590:GLN:HA	1:B:593:GLN:NE2	2.30	0.46
1:E:508:ASN:HD21	1:F:448:LEU:HD23	1.81	0.46
1:K:454:LEU:HD22	1:L:453:PRO:HD3	1.96	0.46
2:2:74:LEU:HD23	2:2:76:LYS:H	1.80	0.46
2:8:27:LEU:HD13	2:8:30:LEU:HD12	1.97	0.46
1:D:394:LEU:HD21	1:D:569:ILE:O	2.14	0.46
1:F:590:GLN:HA	1:F:593:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:400:LYS:O	1:J:404:VAL:HG23	2.15	0.46
1:L:453:PRO:C	1:L:455:ASP:H	2.19	0.46
2:U:5:ALA:HB1	2:U:24:ILE:HG22	1.97	0.46
2:7:74:LEU:HD23	2:7:76:LYS:H	1.81	0.46
1:A:387:TRP:O	1:A:391:VAL:HG23	2.16	0.46
1:C:387:TRP:O	1:C:391:VAL:HG23	2.16	0.46
1:D:508:ASN:HD21	1:E:448:LEU:HD23	1.81	0.46
1:I:508:ASN:HD21	1:J:448:LEU:HD23	1.80	0.46
1:J:303:LEU:H	1:J:303:LEU:HD12	1.80	0.46
1:J:593:GLN:O	1:J:597:VAL:HG23	2.16	0.46
2:5:74:LEU:HD23	2:5:76:LYS:H	1.80	0.46
1:A:389:ALA:HB2	1:A:626:LEU:HD21	1.97	0.46
1:A:550:LYS:HB2	1:A:553:LEU:HD12	1.98	0.46
1:G:447:ALA:HB3	1:L:505:VAL:HB	1.96	0.46
1:H:583:ARG:HA	1:H:584:PRO:HD3	1.82	0.46
1:L:346:ALA:O	1:L:350:VAL:HG23	2.15	0.46
2:9:74:LEU:HD23	2:9:76:LYS:H	1.80	0.46
1:C:583:ARG:HA	1:C:584:PRO:HD3	1.83	0.46
1:G:303:LEU:HD12	1:G:303:LEU:H	1.80	0.46
1:H:409:LEU:O	1:H:413:VAL:HG23	2.14	0.46
1:H:425:LYS:O	1:H:546:ASP:HA	2.16	0.46
1:J:554:LYS:O	1:J:558:GLU:HG3	2.16	0.46
1:L:590:GLN:HA	1:L:593:GLN:NE2	2.31	0.46
2:2:5:ALA:HB1	2:2:24:ILE:HG22	1.98	0.46
2:6:5:ALA:HB1	2:6:24:ILE:HG22	1.98	0.46
2:6:27:LEU:HD13	2:6:30:LEU:HD12	1.98	0.46
2:U:54:LYS:HD3	2:U:61:ILE:HD13	1.98	0.46
2:1:27:LEU:HD13	2:1:30:LEU:HD12	1.97	0.46
2:8:5:ALA:HB1	2:8:24:ILE:HG22	1.98	0.46
1:A:409:LEU:O	1:A:413:VAL:HG23	2.15	0.46
1:G:420:ARG:HB3	1:G:523:PRO:CB	2.44	0.46
1:H:303:LEU:HD12	1:H:303:LEU:H	1.80	0.46
1:H:590:GLN:HA	1:H:593:GLN:NE2	2.31	0.46
1:I:453:PRO:C	1:I:455:ASP:H	2.19	0.46
1:K:409:LEU:O	1:K:413:VAL:HG23	2.15	0.46
2:3:74:LEU:HD23	2:3:76:LYS:H	1.80	0.46
2:U:27:LEU:HD13	2:U:30:LEU:HD12	1.98	0.46
2:U:74:LEU:HD23	2:U:76:LYS:H	1.81	0.46
1:B:439:LEU:HD23	1:B:575:LEU:HD13	1.98	0.46
1:G:425:LYS:O	1:G:546:ASP:HA	2.16	0.46
1:G:590:GLN:HA	1:G:593:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:590:GLN:HA	1:I:593:GLN:NE2	2.31	0.46
1:K:354:GLN:HG2	1:L:310:GLN:HG3	1.97	0.46
1:L:387:TRP:O	1:L:391:VAL:HG23	2.16	0.46
1:L:554:LYS:O	1:L:558:GLU:HG3	2.15	0.46
1:E:409:LEU:O	1:E:413:VAL:HG23	2.14	0.46
1:F:556:CYS:SG	1:F:625:VAL:HG13	2.56	0.46
1:H:387:TRP:O	1:H:391:VAL:HG23	2.15	0.46
1:J:425:LYS:O	1:J:546:ASP:HA	2.16	0.46
1:K:453:PRO:C	1:K:455:ASP:H	2.19	0.46
1:L:420:ARG:HB3	1:L:523:PRO:CB	2.44	0.46
2:W:5:ALA:HB1	2:W:24:ILE:HG22	1.98	0.46
2:W:74:LEU:HD23	2:W:76:LYS:H	1.80	0.46
2:5:27:LEU:HD13	2:5:30:LEU:HD12	1.98	0.46
1:A:286:LEU:HD12	1:F:349:ARG:NH2	2.21	0.45
1:A:590:GLN:HA	1:A:593:GLN:NE2	2.30	0.45
1:D:425:LYS:O	1:D:546:ASP:HA	2.16	0.45
1:D:453:PRO:C	1:D:455:ASP:H	2.19	0.45
1:E:536:THR:HG22	1:F:428:ILE:CG2	2.46	0.45
1:I:409:LEU:O	1:I:413:VAL:HG23	2.15	0.45
1:I:583:ARG:HA	1:I:583:ARG:HD2	1.81	0.45
1:I:621:MET:HB2	1:I:623:ILE:HG12	1.98	0.45
1:L:425:LYS:O	1:L:546:ASP:HA	2.17	0.45
2:4:74:LEU:HD23	2:4:76:LYS:H	1.81	0.45
1:C:391:VAL:HG13	1:C:578:MET:HB2	1.99	0.45
1:F:425:LYS:O	1:F:546:ASP:HA	2.16	0.45
1:F:453:PRO:C	1:F:455:ASP:H	2.19	0.45
1:F:613:GLN:HE21	1:F:613:GLN:N	2.14	0.45
1:G:287:LEU:HD22	1:L:517:ARG:HH12	1.80	0.45
1:H:554:LYS:O	1:H:558:GLU:HG3	2.15	0.45
1:I:425:LYS:O	1:I:546:ASP:HA	2.16	0.45
1:J:439:LEU:HD23	1:J:575:LEU:HD13	1.98	0.45
1:J:590:GLN:HA	1:J:593:GLN:NE2	2.31	0.45
2:6:74:LEU:HD23	2:6:76:LYS:H	1.81	0.45
2:7:27:LEU:HD13	2:7:30:LEU:HD12	1.98	0.45
1:C:550:LYS:HB2	1:C:553:LEU:HD12	1.98	0.45
1:D:556:CYS:SG	1:D:625:VAL:HG13	2.56	0.45
1:H:311:PRO:O	1:H:315:LYS:HB2	2.17	0.45
1:I:556:CYS:SG	1:I:625:VAL:HG13	2.56	0.45
1:I:583:ARG:HA	1:I:584:PRO:HD3	1.83	0.45
1:K:590:GLN:HA	1:K:593:GLN:NE2	2.31	0.45
1:B:425:LYS:O	1:B:546:ASP:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:556:CYS:SG	1:C:625:VAL:HG13	2.56	0.45
1:D:439:LEU:HD23	1:D:575:LEU:HD13	1.98	0.45
1:E:498:ARG:HG3	1:F:474:ASP:CB	2.46	0.45
1:E:556:CYS:SG	1:E:625:VAL:HG13	2.56	0.45
1:F:620:ALA:HB1	2:6:46:ILE:HD12	1.97	0.45
1:G:439:LEU:HD23	1:G:575:LEU:HD13	1.97	0.45
1:H:617:PHE:HZ	2:8:50:THR:HG1	1.64	0.45
2:4:5:ALA:HB1	2:4:24:ILE:HG22	1.98	0.45
1:A:369:LEU:HG	1:A:576:LEU:HD21	1.98	0.45
1:A:425:LYS:O	1:A:546:ASP:HA	2.16	0.45
1:A:433:THR:HG22	1:F:504:SER:HB2	1.98	0.45
1:A:439:LEU:HD23	1:A:575:LEU:HD13	1.97	0.45
1:A:590:GLN:HA	1:A:593:GLN:HE21	1.82	0.45
1:C:453:PRO:C	1:C:455:ASP:H	2.18	0.45
1:F:439:LEU:HD23	1:F:575:LEU:HD13	1.97	0.45
1:F:621:MET:HB2	1:F:623:ILE:HG12	1.99	0.45
1:K:369:LEU:HG	1:K:576:LEU:HD21	1.99	0.45
2:U:34:TYR:CD2	2:U:70:LEU:HD12	2.52	0.45
1:D:303:LEU:HD12	1:D:303:LEU:H	1.79	0.45
1:G:512:LYS:HG3	1:L:514:LEU:HB3	1.97	0.45
1:I:593:GLN:O	1:I:597:VAL:HG23	2.17	0.45
1:J:556:CYS:SG	1:J:625:VAL:HG13	2.57	0.45
2:3:5:ALA:HB1	2:3:24:ILE:HG22	1.99	0.45
1:A:556:CYS:SG	1:A:625:VAL:HG13	2.57	0.45
1:B:556:CYS:SG	1:B:625:VAL:HG13	2.57	0.45
1:D:349:ARG:NH2	1:E:286:LEU:HD12	2.13	0.45
1:G:583:ARG:HA	1:G:584:PRO:HD3	1.83	0.45
1:G:621:MET:HB2	1:G:623:ILE:HG12	1.98	0.45
1:H:439:LEU:HD23	1:H:575:LEU:HD13	1.98	0.45
1:H:556:CYS:SG	1:H:625:VAL:HG13	2.57	0.45
1:I:439:LEU:HD23	1:I:575:LEU:HD13	1.98	0.45
2:3:34:TYR:CD2	2:3:70:LEU:HD12	2.52	0.45
2:W:66:GLU:O	2:W:71:SER:HB3	2.17	0.45
2:4:27:LEU:HD13	2:4:30:LEU:HD12	1.98	0.45
1:G:556:CYS:SG	1:G:625:VAL:HG13	2.56	0.45
1:H:593:GLN:O	1:H:597:VAL:HG23	2.17	0.45
1:L:613:GLN:HE21	1:L:613:GLN:N	2.15	0.45
2:7:5:ALA:HB1	2:7:24:ILE:HG22	1.99	0.45
1:A:621:MET:HB2	1:A:623:ILE:HG12	1.99	0.45
1:B:453:PRO:C	1:B:455:ASP:H	2.19	0.45
1:B:613:GLN:HE21	1:B:613:GLN:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:ARG:HA	1:C:583:ARG:HD2	1.81	0.45
1:C:590:GLN:HA	1:C:593:GLN:NE2	2.31	0.45
1:D:613:GLN:HE21	1:D:613:GLN:N	2.14	0.45
1:H:453:PRO:C	1:H:455:ASP:H	2.19	0.45
1:J:453:PRO:C	1:J:455:ASP:H	2.19	0.45
1:K:439:LEU:HD23	1:K:575:LEU:HD13	1.98	0.45
1:L:593:GLN:O	1:L:597:VAL:HG23	2.17	0.45
2:3:27:LEU:HD13	2:3:30:LEU:HD12	1.98	0.45
2:6:34:TYR:CD2	2:6:70:LEU:HD12	2.52	0.45
2:5:5:ALA:HB1	2:5:24:ILE:HG22	1.99	0.45
1:A:453:PRO:C	1:A:455:ASP:H	2.19	0.45
1:D:504:SER:HB2	1:E:433:THR:HG22	1.98	0.45
1:D:583:ARG:HA	1:D:584:PRO:HD3	1.82	0.45
1:D:590:GLN:HA	1:D:593:GLN:NE2	2.32	0.45
1:E:439:LEU:HD23	1:E:575:LEU:HD13	1.99	0.45
1:G:369:LEU:HG	1:G:576:LEU:HD21	1.99	0.45
1:K:556:CYS:SG	1:K:625:VAL:HG13	2.57	0.45
1:L:439:LEU:HD23	1:L:575:LEU:HD13	1.98	0.45
1:A:420:ARG:HB3	1:A:523:PRO:CB	2.44	0.44
1:G:311:PRO:O	1:G:315:LYS:HB2	2.17	0.44
1:J:583:ARG:HA	1:J:584:PRO:HD3	1.82	0.44
1:K:550:LYS:HB2	1:K:553:LEU:HD12	1.99	0.44
2:2:27:LEU:HD13	2:2:30:LEU:HD12	1.98	0.44
2:3:74:LEU:CD2	2:3:76:LYS:H	2.31	0.44
2:1:34:TYR:CD2	2:1:70:LEU:HD12	2.52	0.44
1:A:276:TYR:HB2	1:A:320:HIS:NE2	2.32	0.44
1:A:459:PHE:HE1	1:B:456:ARG:HE	1.64	0.44
1:C:590:GLN:HA	1:C:593:GLN:HE21	1.82	0.44
1:E:590:GLN:HA	1:E:593:GLN:HE21	1.82	0.44
1:E:613:GLN:HE21	1:E:613:GLN:N	2.14	0.44
1:K:590:GLN:HA	1:K:593:GLN:HE21	1.82	0.44
2:W:34:TYR:CD2	2:W:70:LEU:HD12	2.52	0.44
2:4:34:TYR:CD2	2:4:70:LEU:HD12	2.52	0.44
1:B:311:PRO:O	1:B:315:LYS:HB2	2.17	0.44
1:C:613:GLN:HE21	1:C:613:GLN:N	2.15	0.44
1:C:621:MET:HE1	2:3:46:ILE:HB	1.99	0.44
1:E:449:ASN:HD21	1:E:451:ASN:HB2	1.83	0.44
1:E:621:MET:HB2	1:E:623:ILE:HG12	1.99	0.44
1:F:369:LEU:HG	1:F:576:LEU:HD21	2.00	0.44
1:K:621:MET:HB2	1:K:623:ILE:HG12	1.99	0.44
2:3:66:GLU:O	2:3:71:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:27:LEU:HD13	2:W:30:LEU:HD12	1.98	0.44
2:5:34:TYR:CD2	2:5:70:LEU:HD12	2.53	0.44
2:8:26:LYS:O	2:8:26:LYS:HD3	2.18	0.44
1:A:576:LEU:O	1:A:580:ILE:HG13	2.17	0.44
1:C:311:PRO:O	1:C:315:LYS:HB2	2.17	0.44
1:J:276:TYR:HB2	1:J:320:HIS:NE2	2.33	0.44
1:J:449:ASN:HD21	1:J:451:ASN:HB2	1.82	0.44
1:K:449:ASN:HD21	1:K:451:ASN:HB2	1.83	0.44
1:L:276:TYR:HB2	1:L:320:HIS:NE2	2.32	0.44
1:L:556:CYS:SG	1:L:625:VAL:HG13	2.57	0.44
2:2:66:GLU:O	2:2:71:SER:HB3	2.18	0.44
2:9:34:TYR:CD2	2:9:70:LEU:HD12	2.52	0.44
2:1:74:LEU:CD2	2:1:76:LYS:H	2.31	0.44
1:B:369:LEU:HG	1:B:576:LEU:HD21	1.99	0.44
1:B:590:GLN:HA	1:B:593:GLN:HE21	1.82	0.44
1:C:354:GLN:HG2	1:D:310:GLN:HG3	2.00	0.44
1:C:425:LYS:O	1:C:546:ASP:HA	2.16	0.44
1:C:621:MET:HB2	1:C:623:ILE:HG12	1.98	0.44
1:E:425:LYS:O	1:E:546:ASP:HA	2.17	0.44
1:H:621:MET:HB2	1:H:623:ILE:HG12	1.99	0.44
1:J:621:MET:HB2	1:J:623:ILE:HG12	1.99	0.44
1:K:425:LYS:O	1:K:546:ASP:HA	2.17	0.44
2:2:34:TYR:CD2	2:2:70:LEU:HD12	2.52	0.44
2:1:40:GLY:O	2:1:44:GLU:HG2	2.18	0.44
1:C:576:LEU:O	1:C:580:ILE:HG13	2.17	0.44
1:C:593:GLN:O	1:C:597:VAL:HG23	2.18	0.44
1:E:536:THR:HA	1:F:428:ILE:HG21	2.00	0.44
1:F:449:ASN:HD21	1:F:451:ASN:HB2	1.83	0.44
1:K:613:GLN:HE21	1:K:613:GLN:N	2.16	0.44
2:6:66:GLU:O	2:6:71:SER:HB3	2.18	0.44
2:6:74:LEU:CD2	2:6:76:LYS:H	2.31	0.44
2:W:74:LEU:CD2	2:W:76:LYS:H	2.31	0.44
2:7:34:TYR:CD2	2:7:70:LEU:HD12	2.52	0.44
1:A:311:PRO:O	1:A:315:LYS:HB2	2.18	0.44
1:B:276:TYR:HB2	1:B:320:HIS:NE2	2.33	0.44
1:B:621:MET:HB2	1:B:623:ILE:HG12	1.98	0.44
1:C:454:LEU:HD12	1:C:454:LEU:H	1.82	0.44
1:C:594:SER:O	1:C:598:GLU:HG3	2.18	0.44
1:D:369:LEU:HG	1:D:576:LEU:HD21	2.00	0.44
1:F:550:LYS:HB2	1:F:553:LEU:HD12	2.00	0.44
1:J:613:GLN:HE21	1:J:613:GLN:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:369:LEU:HG	1:L:576:LEU:HD21	2.00	0.44
2:3:40:GLY:O	2:3:44:GLU:HG2	2.18	0.44
2:5:40:GLY:O	2:5:44:GLU:HG2	2.18	0.44
2:5:66:GLU:O	2:5:71:SER:HB3	2.18	0.44
2:1:66:GLU:O	2:1:71:SER:HB3	2.18	0.44
2:8:9:ALA:HA	2:8:12:LEU:HD12	2.00	0.44
1:A:391:VAL:HG13	1:A:578:MET:HB2	1.99	0.44
1:D:276:TYR:HB2	1:D:320:HIS:NE2	2.33	0.44
1:G:339:GLN:NE2	1:H:333:GLN:H	2.16	0.44
1:H:388:MET:HA	1:H:388:MET:HE2	2.00	0.44
1:J:369:LEU:HG	1:J:576:LEU:HD21	2.00	0.44
1:L:621:MET:HB2	1:L:623:ILE:HG12	1.99	0.44
2:9:40:GLY:O	2:9:44:GLU:HG2	2.18	0.44
1:A:454:LEU:HD12	1:A:454:LEU:H	1.83	0.44
1:A:594:SER:O	1:A:598:GLU:HG3	2.18	0.44
1:B:266:LYS:HG3	1:B:267:GLN:H	1.83	0.44
1:B:550:LYS:HB2	1:B:553:LEU:HD12	1.99	0.44
1:E:311:PRO:O	1:E:315:LYS:HB2	2.17	0.44
1:E:593:GLN:O	1:E:597:VAL:HG23	2.17	0.44
1:F:391:VAL:HG13	1:F:578:MET:HB2	2.00	0.44
1:G:473:GLU:CB	1:L:499:ASP:HB3	2.48	0.44
1:G:550:LYS:HB2	1:G:553:LEU:HD12	1.99	0.44
1:I:454:LEU:HD12	1:I:454:LEU:H	1.83	0.44
1:J:311:PRO:O	1:J:315:LYS:HB2	2.17	0.44
1:K:504:SER:O	1:L:437:ALA:HB1	2.18	0.44
2:2:74:LEU:CD2	2:2:76:LYS:H	2.30	0.44
2:5:74:LEU:CD2	2:5:76:LYS:H	2.31	0.44
2:9:27:LEU:HD13	2:9:30:LEU:HD12	1.99	0.44
2:4:74:LEU:CD2	2:4:76:LYS:H	2.31	0.44
1:D:449:ASN:HD21	1:D:451:ASN:HB2	1.83	0.43
1:D:454:LEU:HD12	1:D:454:LEU:H	1.83	0.43
1:E:453:PRO:C	1:E:455:ASP:H	2.19	0.43
1:E:576:LEU:O	1:E:580:ILE:HG13	2.18	0.43
1:H:590:GLN:HA	1:H:593:GLN:HE21	1.83	0.43
1:K:311:PRO:O	1:K:315:LYS:HB2	2.18	0.43
1:K:391:VAL:HG13	1:K:578:MET:HB2	2.00	0.43
1:K:576:LEU:O	1:K:580:ILE:HG13	2.18	0.43
1:L:311:PRO:O	1:L:315:LYS:HB2	2.18	0.43
1:L:391:VAL:HG13	1:L:578:MET:HB2	2.00	0.43
1:L:583:ARG:HA	1:L:584:PRO:HD3	1.82	0.43
2:6:40:GLY:O	2:6:44:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:40:GLY:O	2:4:44:GLU:HG2	2.18	0.43
2:8:34:TYR:CD2	2:8:70:LEU:HD12	2.52	0.43
2:8:40:GLY:O	2:8:44:GLU:HG2	2.18	0.43
1:B:561:GLU:HB3	1:B:565:GLU:OE2	2.18	0.43
1:C:449:ASN:HD21	1:C:451:ASN:HB2	1.83	0.43
1:I:511:LYS:HB3	1:I:516:LYS:HG3	2.01	0.43
2:3:9:ALA:HA	2:3:12:LEU:HD12	2.00	0.43
2:U:26:LYS:HD3	2:U:26:LYS:O	2.19	0.43
2:9:5:ALA:HB1	2:9:24:ILE:HG22	1.99	0.43
2:9:74:LEU:CD2	2:9:76:LYS:H	2.31	0.43
2:1:5:ALA:HB1	2:1:24:ILE:HG22	1.99	0.43
2:1:26:LYS:O	2:1:26:LYS:HD3	2.19	0.43
1:E:550:LYS:HB2	1:E:553:LEU:HD12	1.99	0.43
1:F:276:TYR:HB2	1:F:320:HIS:NE2	2.33	0.43
1:F:311:PRO:O	1:F:315:LYS:HB2	2.17	0.43
1:F:590:GLN:HA	1:F:593:GLN:HE21	1.83	0.43
1:H:276:TYR:HB2	1:H:320:HIS:NE2	2.33	0.43
1:H:369:LEU:HG	1:H:576:LEU:HD21	1.99	0.43
1:H:391:VAL:HG13	1:H:578:MET:HB2	2.00	0.43
1:J:550:LYS:HB2	1:J:553:LEU:HD12	2.00	0.43
1:J:592:ILE:O	1:J:596:ILE:HG12	2.18	0.43
2:W:40:GLY:O	2:W:44:GLU:HG2	2.18	0.43
2:9:66:GLU:O	2:9:71:SER:HB3	2.18	0.43
1:A:499:ASP:HB3	1:B:473:GLU:CB	2.49	0.43
1:B:508:ASN:HD21	1:C:448:LEU:HD23	1.84	0.43
1:B:593:GLN:O	1:B:597:VAL:HG23	2.18	0.43
1:I:276:TYR:HB2	1:I:320:HIS:NE2	2.33	0.43
1:A:593:GLN:O	1:A:597:VAL:HG23	2.18	0.43
1:C:276:TYR:HB2	1:C:320:HIS:NE2	2.33	0.43
1:K:276:TYR:HB2	1:K:320:HIS:NE2	2.33	0.43
1:K:594:SER:O	1:K:598:GLU:HG3	2.18	0.43
1:L:594:SER:O	1:L:598:GLU:HG3	2.19	0.43
2:3:26:LYS:HD3	2:3:26:LYS:O	2.19	0.43
2:6:3:ALA:HB3	2:6:28:VAL:HG13	2.00	0.43
2:U:66:GLU:O	2:U:71:SER:HB3	2.18	0.43
2:W:10:GLU:O	2:W:14:ILE:HG13	2.19	0.43
2:7:9:ALA:HA	2:7:12:LEU:HD12	2.00	0.43
2:8:66:GLU:O	2:8:71:SER:HB3	2.18	0.43
1:B:576:LEU:O	1:B:580:ILE:HG13	2.19	0.43
1:D:593:GLN:O	1:D:597:VAL:HG23	2.18	0.43
1:E:368:LEU:O	1:E:372:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:VAL:HG13	1:E:578:MET:HB2	2.01	0.43
1:H:449:ASN:HD21	1:H:451:ASN:HB2	1.83	0.43
1:H:550:LYS:HB2	1:H:553:LEU:HD12	1.99	0.43
1:I:346:ALA:HB1	1:J:290:GLY:CA	2.48	0.43
1:J:590:GLN:HA	1:J:593:GLN:HE21	1.83	0.43
1:K:454:LEU:HD12	1:K:454:LEU:H	1.83	0.43
1:K:593:GLN:O	1:K:597:VAL:HG23	2.18	0.43
1:L:368:LEU:O	1:L:372:MET:HG3	2.18	0.43
1:L:454:LEU:H	1:L:454:LEU:HD12	1.84	0.43
1:L:590:GLN:HA	1:L:593:GLN:HE21	1.83	0.43
2:8:74:LEU:CD2	2:8:76:LYS:H	2.30	0.43
1:A:449:ASN:HD21	1:A:451:ASN:HB2	1.83	0.43
1:B:449:ASN:HD21	1:B:451:ASN:HB2	1.83	0.43
1:D:592:ILE:O	1:D:596:ILE:HG12	2.19	0.43
1:E:369:LEU:HG	1:E:576:LEU:HD21	1.99	0.43
1:F:594:SER:O	1:F:598:GLU:HG3	2.19	0.43
1:G:449:ASN:HD21	1:G:451:ASN:HB2	1.83	0.43
1:G:504:SER:HB2	1:H:433:THR:HG22	2.00	0.43
1:I:590:GLN:HA	1:I:593:GLN:HE21	1.83	0.43
2:2:26:LYS:O	2:2:26:LYS:HD3	2.19	0.43
2:7:66:GLU:O	2:7:71:SER:HB3	2.18	0.43
2:9:26:LYS:O	2:9:26:LYS:HD3	2.19	0.43
2:1:9:ALA:HA	2:1:12:LEU:HD12	2.00	0.43
1:D:391:VAL:HG13	1:D:578:MET:HB2	2.01	0.43
1:J:350:VAL:HG13	1:K:291:MET:SD	2.59	0.43
1:J:368:LEU:O	1:J:372:MET:HG3	2.19	0.43
2:7:8:LEU:HD23	2:7:8:LEU:O	2.19	0.43
2:7:74:LEU:CD2	2:7:76:LYS:H	2.31	0.43
1:A:592:ILE:O	1:A:596:ILE:HG12	2.19	0.43
1:D:621:MET:HB2	1:D:623:ILE:HG12	1.99	0.43
1:F:454:LEU:HD12	1:F:454:LEU:H	1.84	0.43
1:F:511:LYS:HB3	1:F:516:LYS:HG3	2.01	0.43
1:H:576:LEU:O	1:H:580:ILE:HG13	2.19	0.43
1:I:311:PRO:O	1:I:315:LYS:HB2	2.18	0.43
1:I:620:ALA:HB1	2:9:46:ILE:HD12	2.01	0.43
1:K:389:ALA:HB1	1:K:625:VAL:HG21	2.01	0.43
2:6:57:LEU:HD22	2:6:62:LEU:HD21	2.01	0.43
2:U:40:GLY:O	2:U:44:GLU:HG2	2.18	0.43
2:5:9:ALA:HA	2:5:12:LEU:HD12	2.00	0.43
2:7:40:GLY:O	2:7:44:GLU:HG2	2.19	0.43
1:B:548:ARG:HH12	2:2:7:GLN:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:ARG:HA	1:B:584:PRO:HD3	1.83	0.43
1:D:311:PRO:O	1:D:315:LYS:HB2	2.18	0.43
1:D:396:CYS:HA	2:4:14:ILE:HG23	2.01	0.43
1:D:590:GLN:HA	1:D:593:GLN:HE21	1.84	0.43
1:F:561:GLU:HB3	1:F:565:GLU:OE2	2.19	0.43
1:F:593:GLN:O	1:F:597:VAL:HG23	2.18	0.43
1:G:561:GLU:HB3	1:G:565:GLU:OE2	2.19	0.43
1:G:613:GLN:HE21	1:G:613:GLN:N	2.15	0.43
1:H:368:LEU:O	1:H:372:MET:HG3	2.19	0.43
1:H:613:GLN:HE21	1:H:613:GLN:N	2.16	0.43
1:I:368:LEU:O	1:I:372:MET:HG3	2.18	0.43
1:I:561:GLU:HB3	1:I:565:GLU:OE2	2.19	0.43
1:A:389:ALA:HB1	1:A:625:VAL:HG21	2.01	0.42
1:A:583:ARG:HA	1:A:584:PRO:HD3	1.82	0.42
1:B:592:ILE:O	1:B:596:ILE:HG12	2.19	0.42
1:C:369:LEU:HG	1:C:576:LEU:HD21	2.00	0.42
1:C:372:MET:SD	1:C:576:LEU:HD23	2.59	0.42
1:E:276:TYR:HB2	1:E:320:HIS:NE2	2.33	0.42
1:J:517:ARG:HH12	1:K:287:LEU:HD22	1.84	0.42
2:2:40:GLY:O	2:2:44:GLU:HG2	2.18	0.42
2:6:26:LYS:O	2:6:26:LYS:HD3	2.19	0.42
2:1:10:GLU:O	2:1:14:ILE:HG13	2.19	0.42
2:1:42:VAL:O	2:1:46:ILE:HG13	2.19	0.42
1:E:511:LYS:HB3	1:E:516:LYS:HG3	2.01	0.42
1:G:276:TYR:HB2	1:G:320:HIS:NE2	2.33	0.42
1:G:368:LEU:O	1:G:372:MET:HG3	2.19	0.42
1:G:391:VAL:HG13	1:G:578:MET:HB2	2.00	0.42
1:G:421:TYR:HA	1:G:524:GLY:O	2.19	0.42
1:G:454:LEU:HD12	1:G:454:LEU:H	1.83	0.42
1:G:508:ASN:HD21	1:H:448:LEU:HD23	1.84	0.42
1:G:576:LEU:O	1:G:580:ILE:HG13	2.19	0.42
1:G:621:MET:CE	2:7:46:ILE:HB	2.46	0.42
1:H:389:ALA:HB1	1:H:625:VAL:HG21	2.01	0.42
1:H:508:ASN:HD21	1:I:448:LEU:HD23	1.83	0.42
1:H:511:LYS:HB3	1:H:516:LYS:HG3	2.02	0.42
1:H:592:ILE:O	1:H:596:ILE:HG12	2.20	0.42
1:J:511:LYS:HB3	1:J:516:LYS:HG3	2.01	0.42
1:K:499:ASP:HB3	1:L:473:GLU:HG3	2.01	0.42
2:2:3:ALA:HB3	2:2:28:VAL:HG13	2.02	0.42
2:3:19:CYS:HA	2:3:23:LEU:HD12	2.02	0.42
2:6:42:VAL:O	2:6:46:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:9:ALA:HA	2:U:12:LEU:HD12	2.01	0.42
2:W:26:LYS:O	2:W:26:LYS:HD3	2.19	0.42
2:5:26:LYS:O	2:5:26:LYS:HD3	2.19	0.42
2:9:8:LEU:O	2:9:8:LEU:HD23	2.19	0.42
1:A:310:GLN:HG3	1:F:354:GLN:HG2	2.00	0.42
1:A:613:GLN:HE21	1:A:613:GLN:N	2.16	0.42
1:B:368:LEU:O	1:B:372:MET:HG3	2.20	0.42
1:B:511:LYS:HB3	1:B:516:LYS:HG3	2.02	0.42
1:E:517:ARG:HH12	1:F:287:LEU:HD22	1.85	0.42
1:G:593:GLN:O	1:G:597:VAL:HG23	2.18	0.42
1:H:389:ALA:HB1	1:H:625:VAL:CG2	2.49	0.42
1:I:504:SER:O	1:J:437:ALA:HB1	2.18	0.42
2:U:3:ALA:HB3	2:U:28:VAL:HG13	2.02	0.42
2:7:10:GLU:O	2:7:14:ILE:HG13	2.19	0.42
2:4:66:GLU:O	2:4:71:SER:HB3	2.19	0.42
2:4:67:HIS:HA	2:4:71:SER:HB3	2.02	0.42
1:D:594:SER:O	1:D:598:GLU:HG3	2.20	0.42
1:I:613:GLN:HE21	1:I:613:GLN:N	2.15	0.42
1:K:368:LEU:O	1:K:372:MET:HG3	2.19	0.42
1:K:465:ILE:HG22	1:K:466:ASP:OD2	2.20	0.42
1:K:511:LYS:HB3	1:K:516:LYS:HG3	2.01	0.42
2:U:74:LEU:CD2	2:U:76:LYS:H	2.31	0.42
2:W:9:ALA:HA	2:W:12:LEU:HD12	2.01	0.42
2:5:10:GLU:O	2:5:14:ILE:HG13	2.20	0.42
2:1:57:LEU:HD22	2:1:62:LEU:HD21	2.01	0.42
1:A:389:ALA:HB1	1:A:625:VAL:CG2	2.50	0.42
1:D:550:LYS:HB2	1:D:553:LEU:HD12	2.00	0.42
1:D:561:GLU:HB3	1:D:565:GLU:OE2	2.20	0.42
1:D:576:LEU:O	1:D:580:ILE:HG13	2.20	0.42
1:I:372:MET:SD	1:I:576:LEU:HD23	2.59	0.42
1:I:550:LYS:HB2	1:I:553:LEU:HD12	2.00	0.42
1:J:389:ALA:HB1	1:J:625:VAL:CG2	2.49	0.42
2:2:10:GLU:O	2:2:14:ILE:HG13	2.19	0.42
2:U:67:HIS:HA	2:U:71:SER:HB3	2.02	0.42
2:9:19:CYS:HA	2:9:23:LEU:HD12	2.02	0.42
2:4:3:ALA:HB3	2:4:28:VAL:HG13	2.02	0.42
1:B:391:VAL:HG13	1:B:578:MET:HB2	2.01	0.42
1:B:465:ILE:HG22	1:B:466:ASP:OD2	2.20	0.42
1:C:418:LYS:NZ	1:D:429:ASP:H	2.17	0.42
1:D:368:LEU:O	1:D:372:MET:HG3	2.19	0.42
1:D:511:LYS:HB3	1:D:516:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:454:LEU:H	1:E:454:LEU:HD12	1.84	0.42
1:H:594:SER:O	1:H:598:GLU:HG3	2.19	0.42
1:I:417:PRO:HD3	1:J:567:ARG:HE	1.84	0.42
1:I:449:ASN:HD21	1:I:451:ASN:HB2	1.83	0.42
1:I:594:SER:O	1:I:598:GLU:HG3	2.19	0.42
1:J:354:GLN:HG2	1:K:310:GLN:HG3	2.02	0.42
2:3:3:ALA:HB3	2:3:28:VAL:HG13	2.01	0.42
2:6:10:GLU:O	2:6:14:ILE:HG13	2.20	0.42
2:8:3:ALA:HB3	2:8:28:VAL:HG13	2.01	0.42
1:B:421:TYR:HA	1:B:524:GLY:O	2.19	0.42
1:B:454:LEU:HD12	1:B:454:LEU:H	1.84	0.42
1:B:555:HIS:HA	1:B:558:GLU:OE1	2.20	0.42
1:B:594:SER:O	1:B:598:GLU:HG3	2.19	0.42
1:D:555:HIS:HA	1:D:558:GLU:OE1	2.20	0.42
1:G:555:HIS:HA	1:G:558:GLU:OE1	2.20	0.42
1:H:550:LYS:NZ	2:8:14:ILE:HD13	2.35	0.42
1:I:421:TYR:HA	1:I:524:GLY:O	2.19	0.42
1:I:499:ASP:HB3	1:J:473:GLU:HG3	2.01	0.42
1:I:555:HIS:HA	1:I:558:GLU:OE1	2.20	0.42
1:I:576:LEU:O	1:I:580:ILE:HG13	2.20	0.42
1:J:391:VAL:HG13	1:J:578:MET:HB2	2.01	0.42
1:L:449:ASN:HD21	1:L:451:ASN:HB2	1.84	0.42
2:3:8:LEU:HD23	2:3:8:LEU:O	2.20	0.42
2:U:8:LEU:HD23	2:U:8:LEU:O	2.19	0.42
2:W:19:CYS:HA	2:W:23:LEU:HD12	2.01	0.42
2:9:30:LEU:HB3	2:9:41:MET:SD	2.60	0.42
2:1:3:ALA:HB3	2:1:28:VAL:HG13	2.02	0.42
2:1:8:LEU:O	2:1:8:LEU:HD23	2.20	0.42
2:1:19:CYS:HA	2:1:23:LEU:HD12	2.01	0.42
2:1:20:GLU:H	2:1:23:LEU:HD12	1.85	0.42
2:4:30:LEU:HB3	2:4:41:MET:SD	2.60	0.42
2:8:19:CYS:HA	2:8:23:LEU:HD12	2.02	0.42
1:A:597:VAL:O	1:A:601:GLU:HG3	2.19	0.42
1:B:389:ALA:HB1	1:B:625:VAL:HG21	2.02	0.42
1:C:368:LEU:O	1:C:372:MET:HG3	2.19	0.42
1:C:506:LYS:HA	1:C:520:ILE:HD13	2.02	0.42
1:C:555:HIS:HA	1:C:558:GLU:OE1	2.20	0.42
1:F:368:LEU:O	1:F:372:MET:HG3	2.18	0.42
1:J:561:GLU:HB3	1:J:565:GLU:OE2	2.19	0.42
1:K:421:TYR:HA	1:K:524:GLY:O	2.20	0.42
1:K:422:TRP:CZ3	1:K:543:LYS:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:20:GLU:H	2:2:23:LEU:HD12	1.85	0.42
2:3:67:HIS:HA	2:3:71:SER:HB3	2.01	0.42
2:6:8:LEU:O	2:6:8:LEU:HD23	2.19	0.42
2:W:8:LEU:HD23	2:W:8:LEU:O	2.20	0.42
2:W:67:HIS:HA	2:W:71:SER:HB3	2.02	0.42
2:9:3:ALA:HB3	2:9:28:VAL:HG13	2.01	0.42
2:9:67:HIS:HA	2:9:71:SER:HB3	2.02	0.42
1:A:368:LEU:O	1:A:372:MET:HG3	2.20	0.42
1:A:555:HIS:HA	1:A:558:GLU:OE1	2.19	0.42
1:C:440:LEU:HD13	1:C:471:VAL:HG23	2.02	0.42
1:G:592:ILE:O	1:G:596:ILE:HG12	2.19	0.42
1:I:369:LEU:HG	1:I:576:LEU:HD21	2.00	0.42
1:J:389:ALA:HB1	1:J:625:VAL:HG21	2.01	0.42
1:K:555:HIS:HA	1:K:558:GLU:OE1	2.19	0.42
1:L:576:LEU:O	1:L:580:ILE:HG13	2.19	0.42
1:L:592:ILE:O	1:L:596:ILE:HG12	2.19	0.42
2:3:10:GLU:O	2:3:14:ILE:HG13	2.20	0.42
1:C:561:GLU:HB3	1:C:565:GLU:OE2	2.20	0.42
1:H:372:MET:SD	1:H:576:LEU:HD23	2.60	0.42
1:H:454:LEU:HD12	1:H:454:LEU:H	1.85	0.42
1:I:349:ARG:NH2	1:J:286:LEU:HD12	2.27	0.42
1:I:391:VAL:HG13	1:I:578:MET:HB2	2.01	0.42
1:J:449:ASN:HD22	1:J:452:LEU:HD13	1.85	0.42
1:J:454:LEU:HD12	1:J:454:LEU:H	1.84	0.42
1:K:561:GLU:HB3	1:K:565:GLU:OE2	2.20	0.42
1:L:552:TYR:CE2	2:W:39:GLU:HB3	2.55	0.42
2:2:30:LEU:HB3	2:2:41:MET:SD	2.60	0.42
2:3:20:GLU:H	2:3:23:LEU:HD12	1.84	0.42
2:6:9:ALA:HA	2:6:12:LEU:HD12	2.01	0.42
2:U:20:GLU:H	2:U:23:LEU:HD12	1.85	0.42
2:4:26:LYS:O	2:4:26:LYS:HD3	2.19	0.42
1:B:422:TRP:CZ3	1:B:543:LYS:HD3	2.55	0.41
1:E:389:ALA:HB1	1:E:625:VAL:HG21	2.02	0.41
1:E:443:CYS:HB2	1:E:469:LEU:HD21	2.02	0.41
1:E:594:SER:O	1:E:598:GLU:HG3	2.19	0.41
1:F:576:LEU:O	1:F:580:ILE:HG13	2.19	0.41
1:F:592:ILE:O	1:F:596:ILE:HG12	2.20	0.41
1:G:590:GLN:HA	1:G:593:GLN:HE21	1.84	0.41
1:H:405:VAL:CG1	1:H:579:LEU:HD21	2.50	0.41
1:H:555:HIS:HA	1:H:558:GLU:OE1	2.20	0.41
1:J:405:VAL:CG1	1:J:579:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:389:ALA:HB1	1:L:625:VAL:CG2	2.50	0.41
1:L:597:VAL:O	1:L:601:GLU:HG3	2.20	0.41
2:2:8:LEU:HD23	2:2:8:LEU:O	2.19	0.41
2:U:10:GLU:O	2:U:14:ILE:HG13	2.20	0.41
2:W:3:ALA:HB3	2:W:28:VAL:HG13	2.01	0.41
2:5:19:CYS:HA	2:5:23:LEU:HD12	2.02	0.41
2:5:34:TYR:CE2	2:5:74:LEU:HG	2.55	0.41
2:7:26:LYS:O	2:7:26:LYS:HD3	2.19	0.41
2:9:10:GLU:O	2:9:14:ILE:HG13	2.20	0.41
2:4:9:ALA:HA	2:4:12:LEU:HD12	2.01	0.41
2:8:10:GLU:O	2:8:14:ILE:HG13	2.20	0.41
2:8:30:LEU:HB3	2:8:41:MET:SD	2.60	0.41
1:A:585:VAL:HG21	1:A:597:VAL:HG22	2.02	0.41
1:D:421:TYR:HA	1:D:524:GLY:O	2.20	0.41
1:F:266:LYS:HD2	1:F:266:LYS:N	2.34	0.41
1:F:389:ALA:HB1	1:F:625:VAL:CG2	2.50	0.41
1:G:570:GLN:HE21	1:L:417:PRO:HG2	1.84	0.41
1:G:594:SER:O	1:G:598:GLU:HG3	2.20	0.41
1:H:421:TYR:HA	1:H:524:GLY:O	2.19	0.41
1:I:592:ILE:O	1:I:596:ILE:HG12	2.20	0.41
1:J:594:SER:O	1:J:598:GLU:HG3	2.20	0.41
1:K:597:VAL:O	1:K:601:GLU:HG3	2.20	0.41
1:L:389:ALA:HB1	1:L:625:VAL:HG21	2.02	0.41
1:L:561:GLU:HB3	1:L:565:GLU:OE2	2.20	0.41
2:6:20:GLU:H	2:6:23:LEU:HD12	1.86	0.41
2:1:30:LEU:HB3	2:1:41:MET:SD	2.61	0.41
1:A:421:TYR:HA	1:A:524:GLY:O	2.21	0.41
1:A:561:GLU:HB3	1:A:565:GLU:OE2	2.19	0.41
1:C:511:LYS:HB3	1:C:516:LYS:HG3	2.01	0.41
1:D:389:ALA:HB1	1:D:625:VAL:CG2	2.50	0.41
1:F:372:MET:SD	1:F:576:LEU:HD23	2.61	0.41
1:F:555:HIS:HA	1:F:558:GLU:OE1	2.20	0.41
1:G:389:ALA:HB1	1:G:625:VAL:CG2	2.51	0.41
1:I:389:ALA:HB1	1:I:625:VAL:CG2	2.50	0.41
1:I:389:ALA:HB1	1:I:625:VAL:HG21	2.01	0.41
1:I:449:ASN:HD22	1:I:452:LEU:HD13	1.85	0.41
2:6:30:LEU:HB3	2:6:41:MET:SD	2.61	0.41
2:5:3:ALA:HB3	2:5:28:VAL:HG13	2.02	0.41
2:1:34:TYR:CE2	2:1:74:LEU:HG	2.55	0.41
2:8:34:TYR:CE2	2:8:74:LEU:HG	2.56	0.41
2:8:67:HIS:HA	2:8:71:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ILE:HG22	1:A:466:ASP:OD2	2.20	0.41
1:C:389:ALA:HB1	1:C:625:VAL:CG2	2.51	0.41
1:D:443:CYS:HB2	1:D:469:LEU:HD21	2.02	0.41
1:G:372:MET:SD	1:G:576:LEU:HD23	2.60	0.41
1:G:403:SER:HA	1:G:583:ARG:NH2	2.36	0.41
1:G:449:ASN:HD22	1:G:452:LEU:HD13	1.85	0.41
2:2:19:CYS:HA	2:2:23:LEU:HD12	2.02	0.41
2:3:30:LEU:HB3	2:3:41:MET:SD	2.60	0.41
2:6:67:HIS:HA	2:6:71:SER:HB3	2.02	0.41
2:9:34:TYR:CE2	2:9:74:LEU:HG	2.55	0.41
2:1:67:HIS:HA	2:1:71:SER:HB3	2.01	0.41
2:4:10:GLU:O	2:4:14:ILE:HG13	2.21	0.41
1:A:570:GLN:HE21	1:F:417:PRO:HG2	1.85	0.41
1:C:465:ILE:HG22	1:C:466:ASP:OD2	2.21	0.41
1:E:555:HIS:HA	1:E:558:GLU:OE1	2.20	0.41
1:E:592:ILE:O	1:E:596:ILE:HG12	2.21	0.41
1:F:389:ALA:HB1	1:F:625:VAL:HG21	2.02	0.41
1:G:512:LYS:CD	1:L:514:LEU:HB3	2.51	0.41
1:J:440:LEU:HD13	1:J:471:VAL:HG23	2.02	0.41
1:J:555:HIS:HA	1:J:558:GLU:OE1	2.19	0.41
1:J:584:PRO:HD2	1:J:587:GLU:OE1	2.21	0.41
1:K:389:ALA:HB1	1:K:625:VAL:CG2	2.50	0.41
1:L:405:VAL:CG1	1:L:579:LEU:HD21	2.50	0.41
1:L:555:HIS:HA	1:L:558:GLU:OE1	2.20	0.41
2:3:57:LEU:HD22	2:3:62:LEU:HD21	2.03	0.41
2:6:34:TYR:CE2	2:6:74:LEU:HG	2.56	0.41
2:U:30:LEU:HB3	2:U:41:MET:SD	2.61	0.41
2:W:20:GLU:H	2:W:23:LEU:HD12	1.85	0.41
2:9:9:ALA:HA	2:9:12:LEU:HD12	2.01	0.41
2:4:8:LEU:O	2:4:8:LEU:HD23	2.20	0.41
2:4:20:GLU:H	2:4:23:LEU:HD12	1.85	0.41
1:A:511:LYS:HB3	1:A:516:LYS:HG3	2.02	0.41
1:C:597:VAL:O	1:C:601:GLU:HG3	2.20	0.41
1:E:495:ASP:O	1:E:498:ARG:HG2	2.21	0.41
1:F:583:ARG:HA	1:F:584:PRO:HD3	1.83	0.41
1:F:620:ALA:HB1	2:6:46:ILE:CD1	2.51	0.41
1:G:465:ILE:HG22	1:G:466:ASP:OD2	2.21	0.41
1:H:561:GLU:HB3	1:H:565:GLU:OE2	2.19	0.41
1:J:372:MET:SD	1:J:576:LEU:HD23	2.60	0.41
1:K:388:MET:HE2	1:K:388:MET:HA	2.03	0.41
2:7:34:TYR:CE2	2:7:74:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:20:GLU:H	2:9:23:LEU:HD12	1.85	0.41
2:4:42:VAL:O	2:4:46:ILE:HG13	2.21	0.41
2:8:20:GLU:H	2:8:23:LEU:HD12	1.85	0.41
1:A:611:VAL:O	1:A:615:MET:HG3	2.21	0.41
1:B:372:MET:SD	1:B:576:LEU:HD23	2.61	0.41
1:B:449:ASN:HD22	1:B:452:LEU:HD13	1.85	0.41
1:C:405:VAL:CG1	1:C:579:LEU:HD21	2.50	0.41
1:E:389:ALA:HB1	1:E:625:VAL:CG2	2.50	0.41
1:F:421:TYR:HA	1:F:524:GLY:O	2.20	0.41
1:F:449:ASN:HD22	1:F:452:LEU:HD13	1.85	0.41
1:I:350:VAL:HG13	1:J:291:MET:SD	2.60	0.41
1:J:465:ILE:HG22	1:J:466:ASP:OD2	2.20	0.41
1:L:372:MET:SD	1:L:576:LEU:HD23	2.60	0.41
2:2:57:LEU:HD22	2:2:62:LEU:HD21	2.03	0.41
2:3:34:TYR:CE2	2:3:74:LEU:HG	2.55	0.41
2:W:34:TYR:CE2	2:W:74:LEU:HG	2.55	0.41
2:7:30:LEU:HB3	2:7:41:MET:SD	2.61	0.41
2:4:34:TYR:CE2	2:4:74:LEU:HG	2.56	0.41
1:A:405:VAL:CG1	1:A:579:LEU:HD21	2.50	0.41
1:A:589:ALA:HB3	1:A:592:ILE:HG22	2.03	0.41
1:C:421:TYR:HA	1:C:524:GLY:O	2.20	0.41
1:C:592:ILE:O	1:C:596:ILE:HG12	2.20	0.41
1:D:449:ASN:HD22	1:D:452:LEU:HD13	1.85	0.41
1:F:443:CYS:HB2	1:F:469:LEU:HD21	2.03	0.41
1:G:389:ALA:HB1	1:G:625:VAL:HG21	2.02	0.41
1:G:560:SER:OG	1:G:625:VAL:HG22	2.21	0.41
1:H:443:CYS:HB2	1:H:469:LEU:HD21	2.03	0.41
1:J:403:SER:HA	1:J:583:ARG:NH2	2.35	0.41
1:K:432:LYS:HE3	1:K:529:ASN:HD21	1.86	0.41
1:K:504:SER:HB2	1:L:433:THR:HG22	2.02	0.41
1:L:440:LEU:HD13	1:L:471:VAL:HG23	2.02	0.41
2:U:34:TYR:CE2	2:U:74:LEU:HG	2.56	0.41
2:W:30:LEU:HB3	2:W:41:MET:SD	2.61	0.41
2:7:3:ALA:HB3	2:7:28:VAL:HG13	2.02	0.41
2:7:20:GLU:H	2:7:23:LEU:HD12	1.85	0.41
2:7:67:HIS:HA	2:7:71:SER:HB3	2.02	0.41
2:4:57:LEU:HD22	2:4:62:LEU:HD21	2.02	0.41
1:B:389:ALA:HB1	1:B:625:VAL:CG2	2.51	0.41
1:B:511:LYS:HB3	1:B:516:LYS:HB2	2.03	0.41
1:C:449:ASN:HD22	1:C:452:LEU:HD13	1.86	0.41
1:D:403:SER:HA	1:D:583:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:VAL:CG1	1:D:579:LEU:HD21	2.51	0.41
1:D:506:LYS:HA	1:D:520:ILE:HD13	2.02	0.41
1:E:418:LYS:HE3	1:E:540:ARG:NH1	2.36	0.41
1:E:423:LEU:HB2	1:E:541:PHE:CD2	2.56	0.41
1:E:561:GLU:HB3	1:E:565:GLU:OE2	2.20	0.41
1:G:286:LEU:HB2	1:L:349:ARG:HE	1.86	0.41
1:G:422:TRP:CZ3	1:G:543:LYS:HD3	2.55	0.41
1:G:423:LEU:HB2	1:G:541:PHE:CD2	2.56	0.41
1:G:495:ASP:O	1:G:498:ARG:HG2	2.21	0.41
1:G:597:VAL:O	1:G:601:GLU:HG3	2.21	0.41
1:H:449:ASN:HD22	1:H:452:LEU:HD13	1.86	0.41
1:H:589:ALA:HB3	1:H:592:ILE:HG22	2.03	0.41
1:I:465:ILE:HG22	1:I:466:ASP:OD2	2.21	0.41
1:I:560:SER:OG	1:I:625:VAL:HG22	2.21	0.41
1:J:422:TRP:CZ3	1:J:543:LYS:HD3	2.55	0.41
1:J:576:LEU:O	1:J:580:ILE:HG13	2.20	0.41
1:K:372:MET:SD	1:K:576:LEU:HD23	2.61	0.41
1:K:423:LEU:HB2	1:K:541:PHE:CD2	2.56	0.41
1:K:584:PRO:HD2	1:K:587:GLU:OE1	2.20	0.41
1:L:432:LYS:HE3	1:L:529:ASN:HD21	1.86	0.41
1:L:511:LYS:HB3	1:L:516:LYS:HG3	2.01	0.41
2:2:9:ALA:HA	2:2:12:LEU:HD12	2.03	0.41
2:2:67:HIS:HA	2:2:71:SER:HB3	2.02	0.41
2:6:19:CYS:HA	2:6:23:LEU:HD12	2.02	0.41
2:U:19:CYS:HA	2:U:23:LEU:HD12	2.02	0.41
2:U:42:VAL:O	2:U:46:ILE:HG13	2.21	0.41
2:5:8:LEU:HD23	2:5:8:LEU:O	2.20	0.41
1:A:372:MET:SD	1:A:576:LEU:HD23	2.60	0.41
1:B:403:SER:HA	1:B:583:ARG:NH2	2.35	0.41
1:D:454:LEU:HD12	1:D:454:LEU:N	2.36	0.41
1:F:405:VAL:CG1	1:F:579:LEU:HD21	2.51	0.41
1:F:432:LYS:H	1:F:432:LYS:HG3	1.75	0.41
1:H:465:ILE:HG22	1:H:466:ASP:OD2	2.21	0.41
1:I:405:VAL:CG1	1:I:579:LEU:HD21	2.51	0.41
1:I:584:PRO:HD2	1:I:587:GLU:OE1	2.21	0.41
1:J:479:GLY:HA3	1:J:532:SER:HB3	2.03	0.41
1:J:589:ALA:HB3	1:J:592:ILE:HG22	2.03	0.41
1:K:440:LEU:HD13	1:K:471:VAL:HG23	2.02	0.41
1:K:592:ILE:O	1:K:596:ILE:HG12	2.20	0.41
1:L:465:ILE:HG22	1:L:466:ASP:OD2	2.20	0.41
2:8:8:LEU:HD23	2:8:8:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:GLU:HA	1:A:607:PHE:CZ	2.56	0.40
1:A:422:TRP:CZ3	1:A:543:LYS:HD3	2.56	0.40
1:B:405:VAL:CG1	1:B:579:LEU:HD21	2.51	0.40
1:D:389:ALA:HB1	1:D:625:VAL:HG21	2.02	0.40
1:E:421:TYR:HA	1:E:524:GLY:O	2.20	0.40
1:F:506:LYS:HA	1:F:520:ILE:HD13	2.03	0.40
1:G:511:LYS:HB3	1:G:516:LYS:HG3	2.01	0.40
1:I:418:LYS:HE3	1:I:540:ARG:NH1	2.36	0.40
1:I:440:LEU:HD13	1:I:471:VAL:HG23	2.03	0.40
1:K:508:ASN:HD21	1:L:448:LEU:CD2	2.31	0.40
1:L:584:PRO:HD2	1:L:587:GLU:OE1	2.21	0.40
1:C:423:LEU:HB2	1:C:541:PHE:CD2	2.57	0.40
1:D:372:MET:SD	1:D:576:LEU:HD23	2.62	0.40
1:D:495:ASP:O	1:D:498:ARG:HG2	2.21	0.40
1:H:584:PRO:HD2	1:H:587:GLU:OE1	2.21	0.40
1:I:443:CYS:HB2	1:I:469:LEU:HD21	2.03	0.40
1:K:585:VAL:HG21	1:K:597:VAL:HG22	2.03	0.40
1:L:403:SER:HA	1:L:583:ARG:NH2	2.37	0.40
2:2:34:TYR:CE2	2:2:74:LEU:HG	2.56	0.40
2:W:57:LEU:HD22	2:W:62:LEU:HD21	2.03	0.40
2:5:20:GLU:H	2:5:23:LEU:HD12	1.84	0.40
1:A:448:LEU:HD23	1:F:508:ASN:HD21	1.85	0.40
1:B:440:LEU:HD13	1:B:471:VAL:HG23	2.02	0.40
1:B:506:LYS:HA	1:B:520:ILE:HD13	2.02	0.40
1:E:440:LEU:HD13	1:E:471:VAL:HG23	2.03	0.40
1:F:423:LEU:HB2	1:F:541:PHE:CD2	2.56	0.40
1:H:422:TRP:CZ3	1:H:543:LYS:HD3	2.56	0.40
1:H:440:LEU:HD13	1:H:471:VAL:HG23	2.03	0.40
1:I:495:ASP:O	1:I:498:ARG:HG2	2.22	0.40
1:L:385:GLU:HA	1:L:607:PHE:CZ	2.56	0.40
1:L:443:CYS:HB2	1:L:469:LEU:HD21	2.02	0.40
1:L:506:LYS:HA	1:L:520:ILE:HD13	2.03	0.40
1:A:423:LEU:HB2	1:A:541:PHE:CD2	2.57	0.40
1:B:303:LEU:HD12	1:B:303:LEU:N	2.37	0.40
1:D:388:MET:HA	1:D:388:MET:HE2	2.03	0.40
1:D:422:TRP:CZ3	1:D:543:LYS:HD3	2.56	0.40
1:E:432:LYS:HE3	1:E:529:ASN:HD21	1.86	0.40
1:G:331:LYS:C	1:L:339:GLN:NE2	2.74	0.40
1:I:432:LYS:HE3	1:I:529:ASN:HD21	1.87	0.40
1:I:589:ALA:HB3	1:I:592:ILE:HG22	2.04	0.40
1:K:385:GLU:HA	1:K:607:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:405:VAL:CG1	1:K:579:LEU:HD21	2.51	0.40
1:L:422:TRP:CZ3	1:L:543:LYS:HD3	2.57	0.40
2:5:30:LEU:HB3	2:5:41:MET:SD	2.62	0.40
2:5:67:HIS:HA	2:5:71:SER:HB3	2.02	0.40
1:A:400:LYS:HB3	1:A:403:SER:HB2	2.04	0.40
1:A:443:CYS:HB2	1:A:469:LEU:HD21	2.03	0.40
1:C:443:CYS:HB2	1:C:469:LEU:HD21	2.03	0.40
1:D:385:GLU:HA	1:D:607:PHE:CZ	2.57	0.40
1:D:432:LYS:HE3	1:D:529:ASN:HD21	1.87	0.40
1:E:422:TRP:CZ3	1:E:543:LYS:HD3	2.57	0.40
1:E:449:ASN:HD22	1:E:452:LEU:HD13	1.86	0.40
1:F:440:LEU:HD13	1:F:471:VAL:HG23	2.03	0.40
1:F:465:ILE:HG22	1:F:466:ASP:OD2	2.20	0.40
1:F:511:LYS:HB3	1:F:516:LYS:HB2	2.04	0.40
1:G:433:THR:HG23	1:G:473:GLU:OE1	2.22	0.40
1:G:453:PRO:HD3	1:L:454:LEU:HD22	2.04	0.40
1:I:506:LYS:HA	1:I:520:ILE:HD13	2.03	0.40
1:J:303:LEU:O	1:J:307:LYS:HD3	2.22	0.40
1:K:417:PRO:HG2	1:L:570:GLN:NE2	2.36	0.40
1:L:449:ASN:HD22	1:L:452:LEU:HD13	1.86	0.40
2:7:57:LEU:HD22	2:7:62:LEU:HD21	2.03	0.40
2:9:57:LEU:HD22	2:9:62:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	14 52
1	B	360/362 (99%)	322 (89%)	34 (9%)	4 (1%)	14 52
1	C	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	14 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	14	52
1	E	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	14	52
1	F	360/362 (99%)	322 (89%)	33 (9%)	5 (1%)	11	46
1	G	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	14	52
1	H	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	14	52
1	I	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	14	52
1	J	360/362 (99%)	322 (89%)	33 (9%)	5 (1%)	11	46
1	K	360/362 (99%)	322 (89%)	33 (9%)	5 (1%)	11	46
1	L	360/362 (99%)	323 (90%)	33 (9%)	4 (1%)	14	52
2	1	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	12	48
2	2	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	12	48
2	3	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	12	48
2	4	76/78 (97%)	66 (87%)	9 (12%)	1 (1%)	12	48
2	5	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	12	48
2	6	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	12	48
2	7	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	12	48
2	8	76/78 (97%)	67 (88%)	8 (10%)	1 (1%)	12	48
2	9	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	12	48
2	U	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	12	48
2	W	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	12	48
All	All	5156/5202 (99%)	4617 (90%)	477 (9%)	62 (1%)	13	50

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	474	ASP
1	B	474	ASP
1	C	474	ASP
1	D	474	ASP
1	E	474	ASP
1	F	474	ASP
1	G	474	ASP
1	H	474	ASP
1	I	474	ASP
1	J	474	ASP

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Mol	Chain	Res	Type
1	K	474	ASP
1	L	474	ASP
2	2	4	SER
2	3	4	SER
2	6	4	SER
2	U	4	SER
2	W	4	SER
2	5	4	SER
2	7	4	SER
2	9	4	SER
2	1	4	SER
2	4	4	SER
2	8	4	SER
1	A	429	ASP
1	A	513	HIS
1	B	429	ASP
1	B	513	HIS
1	C	429	ASP
1	C	513	HIS
1	D	429	ASP
1	D	513	HIS
1	E	429	ASP
1	E	513	HIS
1	F	429	ASP
1	F	513	HIS
1	G	429	ASP
1	G	513	HIS
1	H	429	ASP
1	H	513	HIS
1	I	429	ASP
1	I	513	HIS
1	J	267	GLN
1	J	429	ASP
1	J	513	HIS
1	K	429	ASP
1	K	513	HIS
1	L	429	ASP
1	L	513	HIS
1	F	267	GLN
1	K	267	GLN
1	A	523	PRO
1	B	523	PRO

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Mol	Chain	Res	Type
1	C	523	PRO
1	D	523	PRO
1	E	523	PRO
1	F	523	PRO
1	G	523	PRO
1	H	523	PRO
1	I	523	PRO
1	J	523	PRO
1	K	523	PRO
1	L	523	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/323 (100%)	318 (98%)	5 (2%)	65	80
1	B	323/323 (100%)	318 (98%)	5 (2%)	65	80
1	C	323/323 (100%)	317 (98%)	6 (2%)	57	75
1	D	323/323 (100%)	318 (98%)	5 (2%)	65	80
1	E	323/323 (100%)	318 (98%)	5 (2%)	65	80
1	F	323/323 (100%)	318 (98%)	5 (2%)	65	80
1	G	323/323 (100%)	318 (98%)	5 (2%)	65	80
1	H	323/323 (100%)	318 (98%)	5 (2%)	65	80
1	I	323/323 (100%)	316 (98%)	7 (2%)	52	71
1	J	323/323 (100%)	318 (98%)	5 (2%)	65	80
1	K	323/323 (100%)	318 (98%)	5 (2%)	65	80
1	L	323/323 (100%)	318 (98%)	5 (2%)	65	80
2	1	67/67 (100%)	65 (97%)	2 (3%)	41	63
2	2	67/67 (100%)	66 (98%)	1 (2%)	65	80
2	3	67/67 (100%)	65 (97%)	2 (3%)	41	63
2	4	67/67 (100%)	65 (97%)	2 (3%)	41	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	5	67/67 (100%)	65 (97%)	2 (3%)	41	63
2	6	67/67 (100%)	65 (97%)	2 (3%)	41	63
2	7	67/67 (100%)	65 (97%)	2 (3%)	41	63
2	8	67/67 (100%)	65 (97%)	2 (3%)	41	63
2	9	67/67 (100%)	65 (97%)	2 (3%)	41	63
2	U	67/67 (100%)	65 (97%)	2 (3%)	41	63
2	W	67/67 (100%)	65 (97%)	2 (3%)	41	63
All	All	4613/4613 (100%)	4529 (98%)	84 (2%)	59	77

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	CYS
1	A	338	GLN
1	A	415	ASN
1	A	561	GLU
1	A	613	GLN
1	B	302	CYS
1	B	338	GLN
1	B	415	ASN
1	B	561	GLU
1	B	613	GLN
1	C	302	CYS
1	C	338	GLN
1	C	415	ASN
1	C	561	GLU
1	C	583	ARG
1	C	613	GLN
1	D	302	CYS
1	D	338	GLN
1	D	415	ASN
1	D	561	GLU
1	D	613	GLN
1	E	302	CYS
1	E	338	GLN
1	E	415	ASN
1	E	561	GLU
1	E	613	GLN
1	F	302	CYS
1	F	338	GLN

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Mol	Chain	Res	Type
1	F	415	ASN
1	F	561	GLU
1	F	613	GLN
1	G	302	CYS
1	G	338	GLN
1	G	415	ASN
1	G	561	GLU
1	G	613	GLN
1	H	302	CYS
1	H	338	GLN
1	H	415	ASN
1	H	561	GLU
1	H	613	GLN
1	I	266	LYS
1	I	302	CYS
1	I	338	GLN
1	I	415	ASN
1	I	561	GLU
1	I	583	ARG
1	I	613	GLN
1	J	302	CYS
1	J	338	GLN
1	J	415	ASN
1	J	561	GLU
1	J	613	GLN
1	K	302	CYS
1	K	338	GLN
1	K	415	ASN
1	K	561	GLU
1	K	613	GLN
1	L	302	CYS
1	L	338	GLN
1	L	415	ASN
1	L	561	GLU
1	L	613	GLN
2	2	41	MET
2	3	41	MET
2	3	74	LEU
2	6	41	MET
2	6	74	LEU
2	U	41	MET
2	U	74	LEU

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Mol	Chain	Res	Type
2	W	41	MET
2	W	74	LEU
2	5	41	MET
2	5	74	LEU
2	7	41	MET
2	7	74	LEU
2	9	41	MET
2	9	74	LEU
2	1	41	MET
2	1	74	LEU
2	4	41	MET
2	4	74	LEU
2	8	41	MET
2	8	74	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	GLN
1	A	354	GLN
1	A	415	ASN
1	A	449	ASN
1	A	451	ASN
1	A	493	ASN
1	A	508	ASN
1	A	529	ASN
1	A	590	GLN
1	A	593	GLN
1	A	613	GLN
1	B	333	GLN
1	B	354	GLN
1	B	415	ASN
1	B	449	ASN
1	B	451	ASN
1	B	508	ASN
1	B	529	ASN
1	B	590	GLN
1	B	593	GLN
1	B	613	GLN
1	C	333	GLN
1	C	338	GLN
1	C	339	GLN

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Mol	Chain	Res	Type
1	C	354	GLN
1	C	415	ASN
1	C	449	ASN
1	C	451	ASN
1	C	493	ASN
1	C	508	ASN
1	C	529	ASN
1	C	590	GLN
1	C	593	GLN
1	C	613	GLN
1	D	333	GLN
1	D	339	GLN
1	D	415	ASN
1	D	449	ASN
1	D	451	ASN
1	D	493	ASN
1	D	496	ASN
1	D	508	ASN
1	D	529	ASN
1	D	590	GLN
1	D	593	GLN
1	D	613	GLN
1	E	333	GLN
1	E	338	GLN
1	E	415	ASN
1	E	449	ASN
1	E	451	ASN
1	E	493	ASN
1	E	508	ASN
1	E	529	ASN
1	E	590	GLN
1	E	593	GLN
1	E	613	GLN
1	F	333	GLN
1	F	338	GLN
1	F	339	GLN
1	F	354	GLN
1	F	415	ASN
1	F	449	ASN
1	F	451	ASN
1	F	493	ASN
1	F	496	ASN

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Mol	Chain	Res	Type
1	F	508	ASN
1	F	529	ASN
1	F	590	GLN
1	F	593	GLN
1	F	613	GLN
1	G	333	GLN
1	G	338	GLN
1	G	339	GLN
1	G	354	GLN
1	G	415	ASN
1	G	449	ASN
1	G	451	ASN
1	G	493	ASN
1	G	496	ASN
1	G	508	ASN
1	G	513	HIS
1	G	529	ASN
1	G	590	GLN
1	G	593	GLN
1	G	613	GLN
1	H	333	GLN
1	H	338	GLN
1	H	339	GLN
1	H	354	GLN
1	H	415	ASN
1	H	449	ASN
1	H	451	ASN
1	H	493	ASN
1	H	496	ASN
1	H	508	ASN
1	H	529	ASN
1	H	590	GLN
1	H	593	GLN
1	H	613	GLN
1	I	333	GLN
1	I	339	GLN
1	I	415	ASN
1	I	449	ASN
1	I	451	ASN
1	I	493	ASN
1	I	508	ASN
1	I	529	ASN

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Mol	Chain	Res	Type
1	I	590	GLN
1	I	593	GLN
1	I	613	GLN
1	J	333	GLN
1	J	338	GLN
1	J	339	GLN
1	J	354	GLN
1	J	415	ASN
1	J	449	ASN
1	J	451	ASN
1	J	493	ASN
1	J	496	ASN
1	J	508	ASN
1	J	529	ASN
1	J	590	GLN
1	J	593	GLN
1	J	613	GLN
1	K	333	GLN
1	K	339	GLN
1	K	354	GLN
1	K	415	ASN
1	K	449	ASN
1	K	451	ASN
1	K	493	ASN
1	K	508	ASN
1	K	513	HIS
1	K	529	ASN
1	K	590	GLN
1	K	593	GLN
1	K	613	GLN
1	L	333	GLN
1	L	339	GLN
1	L	415	ASN
1	L	449	ASN
1	L	451	ASN
1	L	493	ASN
1	L	496	ASN
1	L	508	ASN
1	L	513	HIS
1	L	529	ASN
1	L	590	GLN
1	L	593	GLN

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Mol	Chain	Res	Type
1	L	613	GLN
2	2	7	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	362/362 (100%)	0.48	22 (6%)	21	17	262, 300, 300, 300	0
1	B	362/362 (100%)	0.30	8 (2%)	62	52	260, 300, 300, 300	0
1	C	362/362 (100%)	0.37	8 (2%)	62	52	260, 300, 300, 300	0
1	D	362/362 (100%)	0.29	9 (2%)	57	48	257, 300, 300, 300	0
1	E	362/362 (100%)	0.35	7 (1%)	66	58	260, 300, 300, 300	0
1	F	362/362 (100%)	0.38	9 (2%)	57	48	258, 300, 300, 300	0
1	G	362/362 (100%)	0.47	20 (5%)	25	22	260, 300, 300, 300	0
1	H	362/362 (100%)	0.31	11 (3%)	50	40	260, 300, 300, 300	0
1	I	362/362 (100%)	0.33	14 (3%)	39	32	260, 300, 300, 300	0
1	J	362/362 (100%)	0.34	10 (2%)	53	43	261, 300, 300, 300	0
1	K	362/362 (100%)	0.35	9 (2%)	57	48	260, 300, 300, 300	0
1	L	362/362 (100%)	0.32	13 (3%)	42	35	262, 300, 300, 300	0
2	1	78/78 (100%)	1.24	19 (24%)	0	1	281, 300, 300, 300	0
2	2	78/78 (100%)	0.73	10 (12%)	3	5	278, 300, 300, 300	0
2	3	78/78 (100%)	0.92	13 (16%)	1	3	280, 300, 300, 300	0
2	4	78/78 (100%)	1.38	24 (30%)	0	1	281, 300, 300, 300	0
2	5	78/78 (100%)	1.10	19 (24%)	0	1	281, 300, 300, 300	0
2	6	78/78 (100%)	1.18	17 (21%)	0	1	281, 300, 300, 300	0
2	7	78/78 (100%)	0.88	12 (15%)	2	3	280, 300, 300, 300	0
2	8	78/78 (100%)	1.40	24 (30%)	0	1	280, 300, 300, 300	0
2	9	78/78 (100%)	1.12	17 (21%)	0	1	280, 300, 300, 300	0
2	U	78/78 (100%)	1.28	18 (23%)	0	1	280, 300, 300, 300	0
2	W	78/78 (100%)	0.88	9 (11%)	4	6	279, 300, 300, 300	0
All	All	5202/5202 (100%)	0.48	322 (6%)	20	17	257, 300, 300, 300	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	1	1	MET	8.4
2	1	78	ARG	7.2
2	1	2	SER	6.8
2	6	78	ARG	6.3
2	5	78	ARG	6.2
2	3	2	SER	6.1
2	2	78	ARG	6.0
2	4	57	LEU	5.9
2	6	57	LEU	5.8
2	5	2	SER	5.6
2	4	77	ALA	5.6
2	4	56	GLY	5.6
2	9	78	ARG	5.5
2	7	1	MET	5.5
2	U	78	ARG	5.5
2	7	2	SER	5.5
2	W	1	MET	5.4
2	U	76	LYS	5.3
2	U	57	LEU	5.2
2	U	75	SER	5.2
2	1	75	SER	5.2
2	4	75	SER	5.2
2	1	73	ARG	4.9
2	3	78	ARG	4.9
2	U	74	LEU	4.8
1	H	266	LYS	4.8
2	9	2	SER	4.7
2	7	78	ARG	4.7
2	4	3	ALA	4.7
2	3	1	MET	4.7
2	8	56	GLY	4.7
2	9	66	GLU	4.6
2	1	11	GLU	4.6
2	8	33	GLN	4.6
1	A	396	CYS	4.6
2	6	1	MET	4.6
2	U	2	SER	4.5
1	J	532	SER	4.5
2	9	77	ALA	4.5
2	7	77	ALA	4.4
2	4	78	ARG	4.4
2	6	56	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
2	4	76	LYS	4.2
2	8	2	SER	4.2
2	8	75	SER	4.1
2	W	2	SER	4.1
2	8	1	MET	4.1
2	6	2	SER	4.0
2	3	76	LYS	4.0
2	8	57	LEU	4.0
2	9	76	LYS	4.0
2	4	2	SER	3.9
2	8	15	PHE	3.9
2	4	74	LEU	3.9
2	9	1	MET	3.9
2	3	75	SER	3.8
2	2	77	ALA	3.8
2	U	66	GLU	3.8
2	U	1	MET	3.8
1	C	266	LYS	3.8
1	L	293	LEU	3.8
2	9	3	ALA	3.6
2	8	73	ARG	3.6
2	6	76	LYS	3.6
2	W	77	ALA	3.6
2	8	32	VAL	3.6
2	1	69	PHE	3.6
2	7	76	LYS	3.6
2	3	3	ALA	3.6
1	D	292	TYR	3.5
1	G	581	TRP	3.5
2	1	15	PHE	3.5
2	5	3	ALA	3.5
2	8	61	ILE	3.5
2	4	62	LEU	3.5
2	6	58	THR	3.5
2	9	74	LEU	3.5
1	E	513	HIS	3.4
2	5	77	ALA	3.4
2	8	62	LEU	3.4
1	I	536	THR	3.4
2	U	36	GLN	3.4
2	6	74	LEU	3.4
2	3	57	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	513	HIS	3.4
1	K	293	LEU	3.4
1	J	536	THR	3.4
2	1	77	ALA	3.4
2	6	15	PHE	3.3
1	A	388	MET	3.3
2	9	75	SER	3.3
2	1	74	LEU	3.3
1	A	392	ALA	3.3
2	8	76	LYS	3.3
2	3	56	GLY	3.3
2	W	66	GLU	3.3
2	5	76	LYS	3.2
1	B	337	CYS	3.2
1	I	292	TYR	3.2
2	U	56	GLY	3.2
2	6	77	ALA	3.2
2	6	73	ARG	3.2
2	2	76	LYS	3.1
1	F	292	TYR	3.1
2	3	77	ALA	3.1
2	2	75	SER	3.1
1	L	378	SER	3.1
2	6	19	CYS	3.1
1	A	296	GLN	3.1
2	U	77	ALA	3.1
1	D	607	PHE	3.1
1	A	569	ILE	3.1
2	8	35	GLY	3.1
1	A	333	GLN	3.1
1	J	531	TYR	3.0
1	I	513	HIS	3.0
2	4	14	ILE	3.0
1	K	581	TRP	3.0
2	6	75	SER	3.0
2	1	3	ALA	3.0
1	F	508	ASN	3.0
1	H	426	GLY	3.0
2	2	2	SER	3.0
2	9	73	ARG	2.9
1	K	354	GLN	2.9
1	F	616	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	7	34	TYR	2.9
1	G	273	VAL	2.9
1	G	513	HIS	2.9
1	A	612	TYR	2.9
1	I	268	VAL	2.9
2	4	70	LEU	2.9
1	K	266	LYS	2.8
1	H	607	PHE	2.8
2	1	66	GLU	2.8
1	L	333	GLN	2.8
2	7	75	SER	2.8
2	1	76	LYS	2.8
2	9	34	TYR	2.8
1	G	268	VAL	2.8
2	4	26	LYS	2.8
1	B	626	LEU	2.8
2	5	19	CYS	2.8
1	I	267	GLN	2.8
2	1	70	LEU	2.8
2	7	33	GLN	2.8
2	4	33	GLN	2.8
2	7	18	ASP	2.8
1	L	292	TYR	2.8
1	I	296	GLN	2.8
1	J	479	GLY	2.8
1	G	479	GLY	2.7
1	H	267	GLN	2.7
1	J	540	ARG	2.7
1	H	599	TRP	2.7
2	9	70	LEU	2.7
1	C	625	VAL	2.7
2	5	41	MET	2.7
1	I	318	GLU	2.7
2	2	66	GLU	2.7
1	K	319	LYS	2.7
2	8	51	SER	2.7
1	H	292	TYR	2.7
1	C	318	GLU	2.6
2	W	52	THR	2.6
2	2	15	PHE	2.6
2	U	73	ARG	2.6
2	U	35	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	8	58	THR	2.6
1	G	536	THR	2.6
1	G	292	TYR	2.6
1	G	386	GLU	2.6
2	U	37	ASN	2.6
1	C	626	LEU	2.6
2	U	15	PHE	2.6
2	U	41	MET	2.6
1	E	530	GLU	2.5
2	3	74	LEU	2.5
2	4	66	GLU	2.5
1	K	296	GLN	2.5
1	I	327	PHE	2.5
2	2	1	MET	2.5
2	4	34	TYR	2.5
2	9	57	LEU	2.5
2	4	58	THR	2.5
1	A	329	ASP	2.5
1	L	354	GLN	2.5
2	5	72	LYS	2.5
1	B	268	VAL	2.5
1	A	599	TRP	2.5
2	8	74	LEU	2.5
1	A	330	SER	2.5
1	E	266	LYS	2.5
2	5	56	GLY	2.5
1	I	333	GLN	2.5
2	5	8	LEU	2.5
2	8	78	ARG	2.5
2	3	17	LEU	2.5
1	K	292	TYR	2.4
2	5	66	GLU	2.4
2	5	74	LEU	2.4
2	4	35	GLY	2.4
1	E	510	GLU	2.4
2	5	75	SER	2.4
2	4	71	SER	2.4
2	7	3	ALA	2.4
2	8	31	CYS	2.4
2	8	3	ALA	2.4
1	A	391	VAL	2.4
1	D	513	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	W	42	VAL	2.4
1	G	445	GLY	2.4
2	7	74	LEU	2.4
1	C	615	MET	2.4
2	1	72	LYS	2.4
1	C	515	ASN	2.4
1	H	396	CYS	2.4
1	A	616	LYS	2.4
2	8	36	GLN	2.4
1	G	532	SER	2.3
1	F	625	VAL	2.3
2	9	62	LEU	2.3
2	8	70	LEU	2.3
1	I	602	ARG	2.3
1	J	612	TYR	2.3
1	K	318	GLU	2.3
1	K	532	SER	2.3
1	B	267	GLN	2.3
1	J	513	HIS	2.3
1	G	318	GLU	2.3
1	H	385	GLU	2.3
1	G	387	TRP	2.3
2	5	57	LEU	2.3
1	A	460	GLU	2.3
1	A	327	PHE	2.3
1	F	607	PHE	2.3
2	2	52	THR	2.3
1	A	568	ILE	2.3
1	J	388	MET	2.3
1	I	396	CYS	2.3
2	5	34	TYR	2.3
2	6	70	LEU	2.3
1	C	327	PHE	2.3
1	G	529	ASN	2.3
1	H	388	MET	2.2
1	L	379	THR	2.2
1	D	388	MET	2.2
2	1	57	LEU	2.2
1	D	581	TRP	2.2
1	E	447	ALA	2.2
1	L	626	LEU	2.2
1	G	580	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	3	62	LEU	2.2
1	J	581	TRP	2.2
1	A	626	LEU	2.2
2	4	32	VAL	2.2
1	D	596	ILE	2.2
1	G	540	ARG	2.2
2	4	5	ALA	2.2
1	L	531	TYR	2.2
2	2	74	LEU	2.2
2	6	36	GLN	2.2
2	8	66	GLU	2.2
1	B	336	ILE	2.2
1	A	292	TYR	2.2
1	A	607	PHE	2.2
2	8	72	LYS	2.2
1	G	331	LYS	2.2
1	I	354	GLN	2.2
1	E	292	TYR	2.1
2	5	1	MET	2.1
2	9	72	LYS	2.1
1	L	486	PRO	2.1
2	7	66	GLU	2.1
1	J	607	PHE	2.1
2	5	70	LEU	2.1
1	D	532	SER	2.1
2	9	38	GLU	2.1
1	D	445	GLY	2.1
2	U	19	CYS	2.1
1	G	267	GLN	2.1
1	B	596	ILE	2.1
1	A	562	PHE	2.1
2	3	33	GLN	2.1
1	E	529	ASN	2.1
1	I	484	ASP	2.1
2	9	8	LEU	2.1
1	G	577	LEU	2.1
2	6	34	TYR	2.1
2	4	31	CYS	2.1
1	G	625	VAL	2.1
1	A	320	HIS	2.1
1	H	536	THR	2.1
1	F	512	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	4	36	GLN	2.1
2	6	66	GLU	2.1
1	L	495	ASP	2.1
1	G	518	THR	2.1
1	L	580	ILE	2.1
2	5	36	GLN	2.1
1	F	293	LEU	2.0
1	F	379	THR	2.0
2	1	45	LEU	2.0
2	U	3	ALA	2.0
1	B	607	PHE	2.0
2	W	53	HIS	2.0
1	B	283	ASP	2.0
1	D	544	GLN	2.0
2	5	18	ASP	2.0
2	8	71	SER	2.0
2	W	26	LYS	2.0
2	1	14	ILE	2.0
2	4	15	PHE	2.0
1	F	626	LEU	2.0
1	A	270	TRP	2.0
1	A	581	TRP	2.0
1	H	300	GLU	2.0
1	L	289	LEU	2.0
1	L	296	GLN	2.0
2	W	78	ARG	2.0
1	I	294	GLU	2.0
2	1	42	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	C	700	1/1	0.45	0.17	300,300,300,300	0
3	ZN	K	700	1/1	0.52	0.15	300,300,300,300	0
3	ZN	F	700	1/1	0.65	0.09	300,300,300,300	0
3	ZN	H	700	1/1	0.70	0.10	300,300,300,300	0
3	ZN	I	700	1/1	0.75	0.12	300,300,300,300	0
3	ZN	G	700	1/1	0.76	0.14	300,300,300,300	0
3	ZN	E	700	1/1	0.79	0.16	300,300,300,300	0
3	ZN	B	700	1/1	0.83	0.17	300,300,300,300	0
3	ZN	A	700	1/1	0.91	0.08	300,300,300,300	0
3	ZN	D	700	1/1	0.92	0.05	245,245,245,245	0
3	ZN	J	700	1/1	0.94	0.10	300,300,300,300	0
3	ZN	L	700	1/1	0.97	0.04	300,300,300,300	0

6.5 Other polymers (i)

There are no such residues in this entry.