Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 04:34 PM EST

PDB ID	:	3PU0
Title	:	Crystal Structure of a vesicular stomatitis virus nucleocapsid-polyC complex
Authors	:	Luo, M.; Green, T.J.; Rowse, M.
Deposited on	:	2010-12-03
Resolution	:	3.09 Å(reported)

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

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

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

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

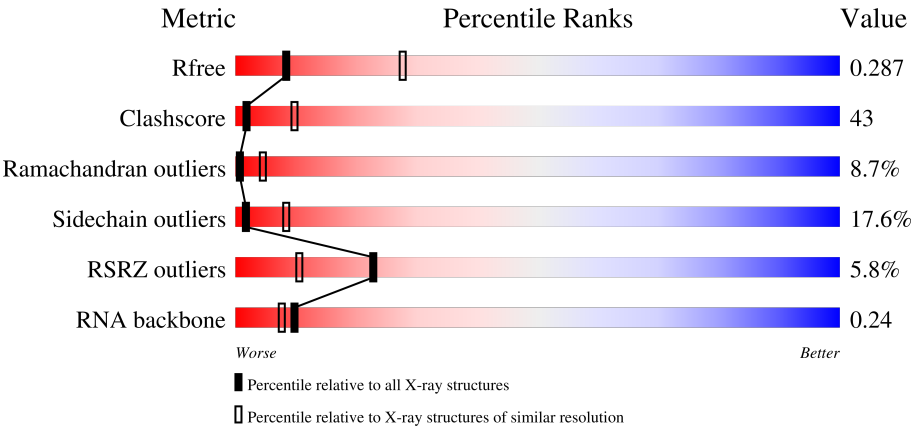
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.09 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	421	8% 43% 43% 13%
1	B	421	3% 40% 43% 14%
1	C	421	5% 42% 40% 14%
1	D	421	5% 42% 42% 13%

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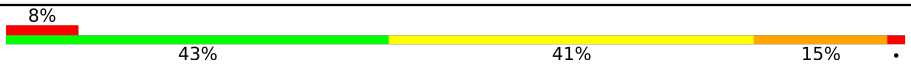
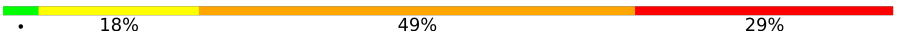
Mol	Chain	Length	Quality of chain
1	E	421	
2	R	45	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17437 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

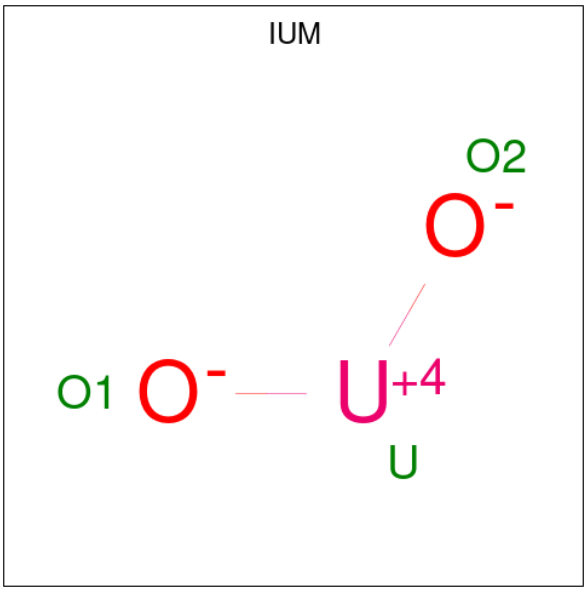
- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	B	415	Total	C	N	O	S	0	0	0
			3290	2097	552	623	18			
1	C	413	Total	C	N	O	S	0	0	0
			3275	2089	550	618	18			
1	D	416	Total	C	N	O	S	0	0	0
			3298	2103	553	624	18			
1	E	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			

- Molecule 2 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	45	Total	C	N	O	P	0	0	0
			900	405	135	315	45			

- Molecule 3 is URANYL (VI) ION (three-letter code: IUM) (formula: O_2U).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total U 1 1	0	0
3	A	1	Total U 1 1	0	0
3	A	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	C	1	Total U 1 1	0	0
3	C	1	Total U 1 1	0	0
3	D	1	Total U 1 1	0	0
3	D	1	Total U 1 1	0	0
3	D	1	Total U 1 1	0	0
3	E	1	Total U 1 1	0	0
3	E	1	Total U 1 1	0	0

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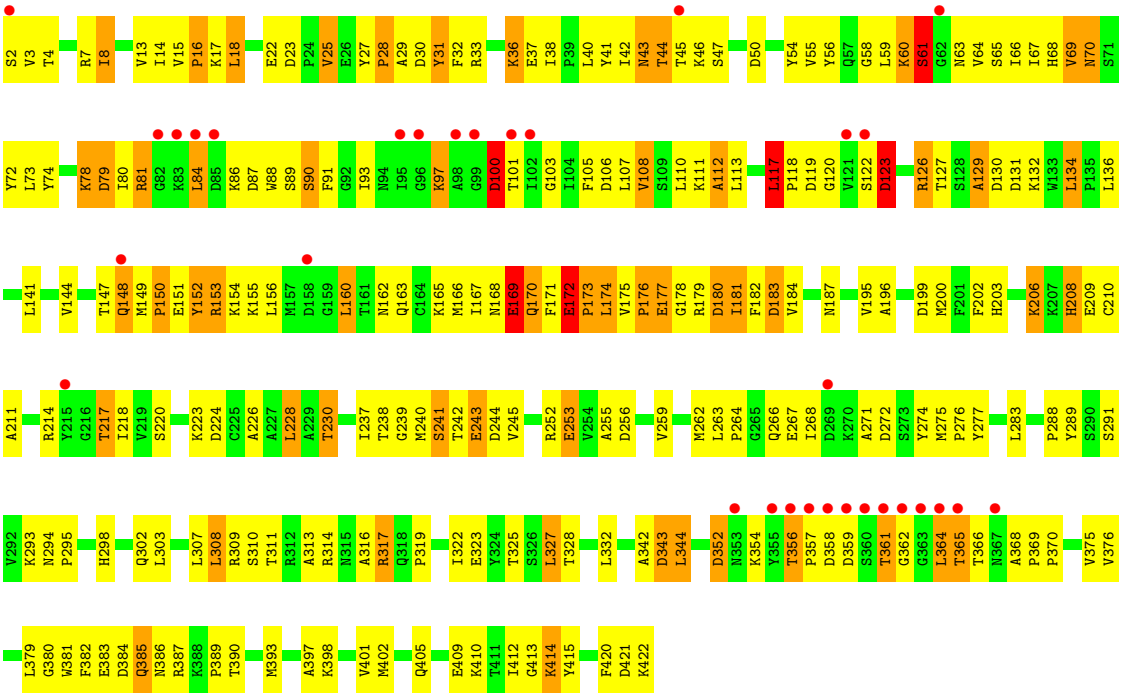
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0

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.

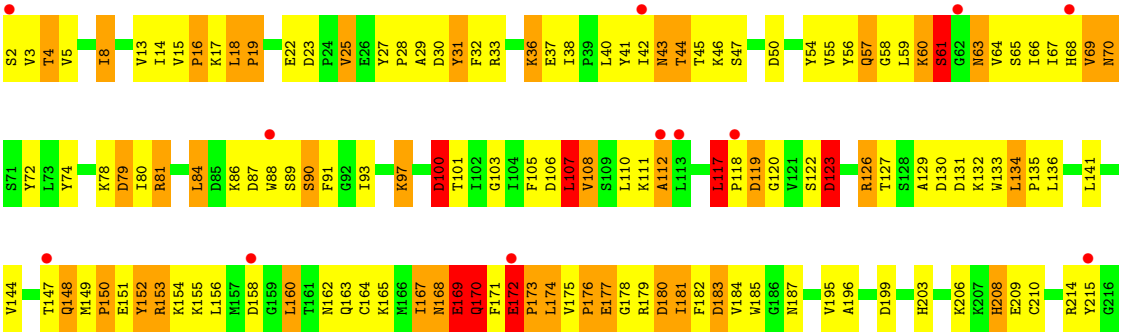
• Molecule 1: Nucleoprotein

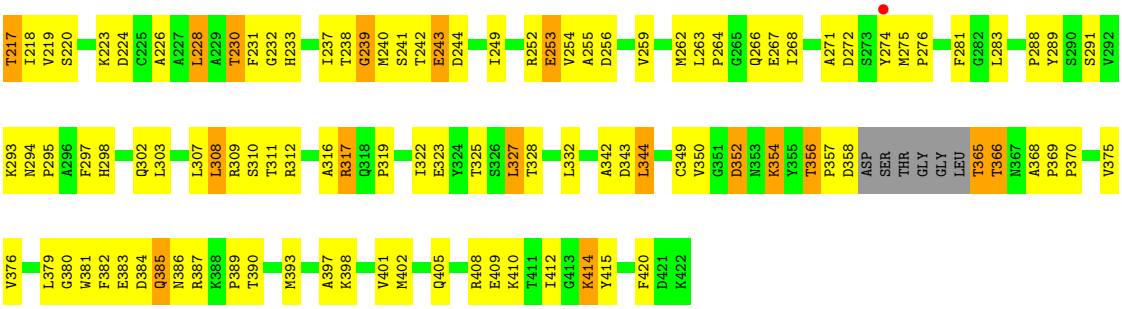
Chain A:



• Molecule 1: Nucleoprotein

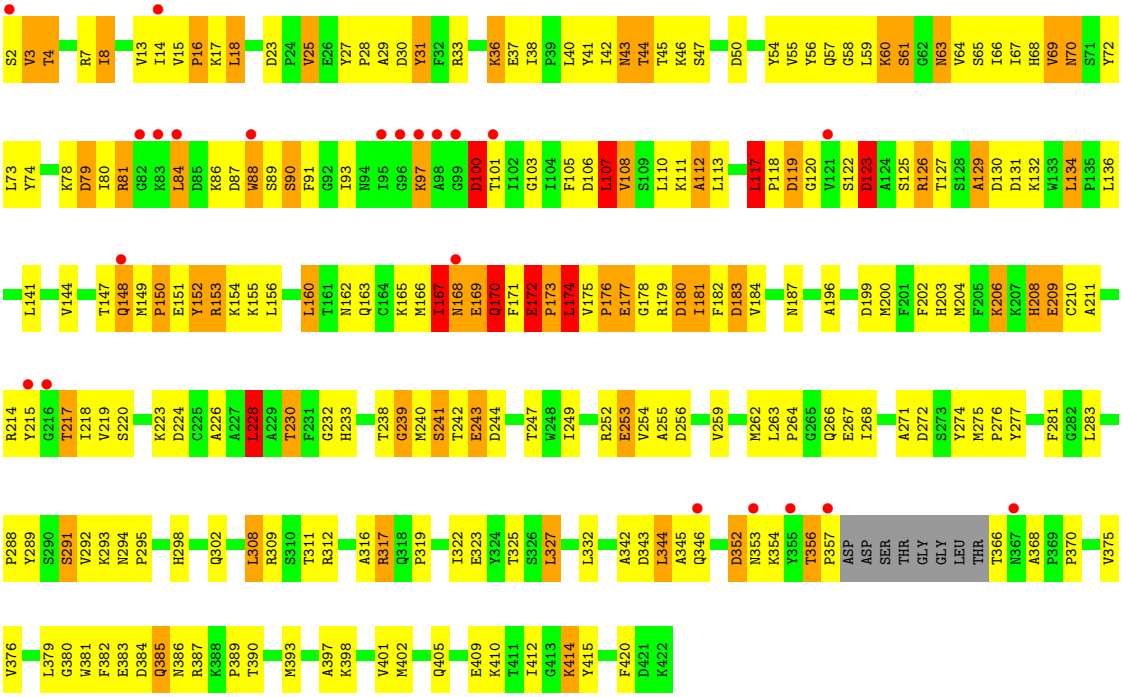
Chain B:





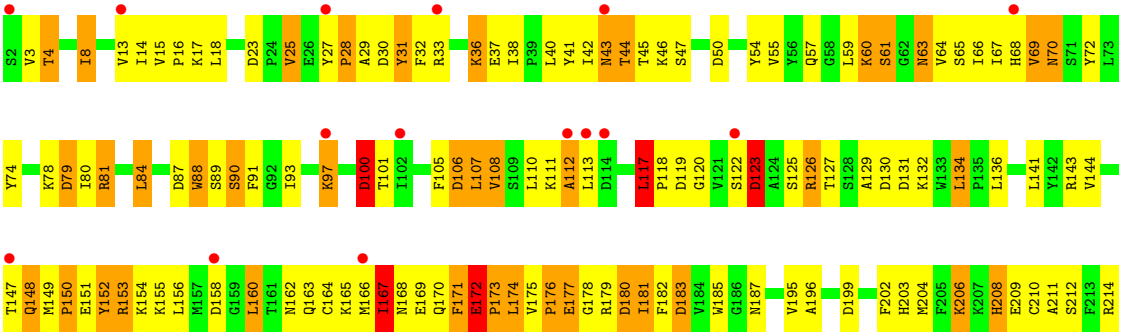
• Molecule 1: Nucleoprotein

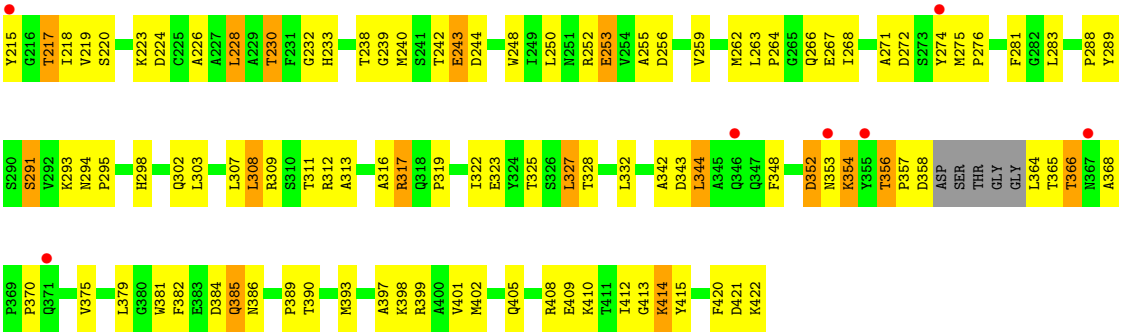
Chain C:



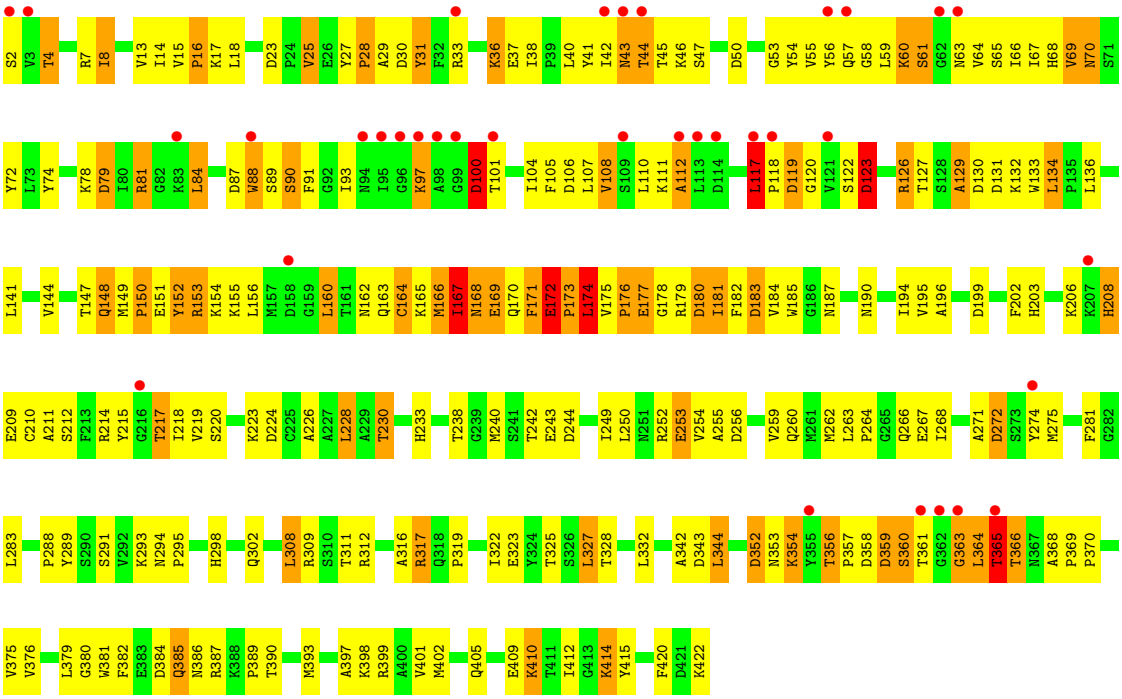
• Molecule 1: Nucleoprotein

Chain D:

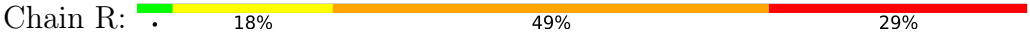


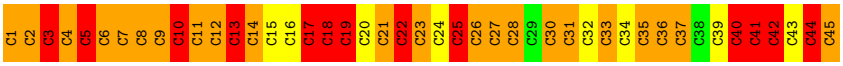


• Molecule 1: Nucleoprotein



• Molecule 2: RNA (45-MER)





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	164.65Å 235.55Å 75.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.09 49.75 – 3.09	Depositor EDS
% Data completeness (in resolution range)	78.5 (49.75-3.09) 78.5 (49.75-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.16 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.6_289	Depositor
R, R_{free}	0.250 , 0.290 0.241 , 0.287	Depositor DCC
R_{free} test set	2000 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å^2)	73.2	Xtriage
Anisotropy	0.879	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	17437	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.51	0/3403	0.67	1/4607 (0.0%)
1	B	0.51	0/3365	0.65	1/4554 (0.0%)
1	C	0.52	0/3350	0.65	0/4533
1	D	0.53	0/3373	0.65	0/4565
1	E	0.52	0/3403	0.66	0/4607
2	R	0.91	0/989	2.08	59/1526 (3.9%)
All	All	0.55	0/17883	0.82	61/24392 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	1
1	D	0	1
1	E	0	3
All	All	0	11

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	27	C	O4'-C1'-N1	11.92	117.74	108.20
2	R	18	C	N1-C1'-C2'	-11.43	99.14	114.00
2	R	15	C	N1-C1'-C2'	9.61	126.49	114.00
2	R	4	C	O4'-C1'-N1	9.18	115.54	108.20
2	R	9	C	O4'-C1'-N1	8.91	115.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	26	C	O4'-C1'-N1	8.35	114.88	108.20
2	R	37	C	O4'-C1'-N1	7.88	114.50	108.20
2	R	27	C	N1-C2-O2	7.78	123.57	118.90
2	R	41	C	N1-C1'-C2'	-7.76	103.47	112.00
2	R	22	C	O4'-C1'-N1	7.62	114.30	108.20
2	R	35	C	O4'-C1'-N1	7.48	114.19	108.20
2	R	6	C	C6-N1-C2	-7.39	117.34	120.30
2	R	44	C	O4'-C1'-N1	7.39	114.11	108.20
2	R	2	C	P-O3'-C3'	-7.30	110.94	119.70
2	R	36	C	O4'-C1'-N1	7.27	114.02	108.20
1	A	61	SER	CB-CA-C	7.21	123.81	110.10
2	R	4	C	P-O3'-C3'	-7.15	111.12	119.70
2	R	43	C	P-O3'-C3'	7.06	128.17	119.70
2	R	30	C	O4'-C1'-N1	-6.95	102.64	108.20
2	R	9	C	N1-C2-O2	6.78	122.97	118.90
2	R	6	C	N1-C1'-C2'	6.61	122.60	114.00
2	R	15	C	N1-C2-O2	6.56	122.83	118.90
2	R	41	C	C6-N1-C2	-6.45	117.72	120.30
2	R	15	C	N3-C2-O2	-6.38	117.43	121.90
2	R	20	C	P-O3'-C3'	-6.35	112.08	119.70
1	B	61	SER	CB-CA-C	6.32	122.11	110.10
2	R	21	C	O4'-C1'-N1	-6.25	103.20	108.20
2	R	8	C	P-O3'-C3'	6.23	127.18	119.70
2	R	25	C	O4'-C1'-N1	6.20	113.16	108.20
2	R	10	C	C5-C6-N1	6.19	124.10	121.00
2	R	41	C	C3'-C2'-C1'	6.18	106.45	101.50
2	R	33	C	O4'-C1'-N1	-6.14	103.29	108.20
2	R	17	C	N1-C1'-C2'	5.99	121.78	114.00
2	R	13	C	O4'-C1'-N1	5.98	112.98	108.20
2	R	3	C	O4'-C1'-N1	-5.96	103.43	108.20
2	R	11	C	P-O5'-C5'	5.90	130.34	120.90
2	R	7	C	O4'-C1'-N1	-5.88	103.49	108.20
2	R	19	C	P-O3'-C3'	-5.71	112.84	119.70
2	R	33	C	N1-C2-O2	5.67	122.30	118.90
2	R	9	C	N3-C2-O2	-5.62	117.96	121.90
2	R	5	C	N1-C1'-C2'	5.57	121.24	114.00
2	R	1	C	P-O3'-C3'	5.53	126.33	119.70
2	R	33	C	N1-C1'-C2'	5.43	121.06	114.00
2	R	27	C	O3'-P-O5'	-5.42	93.70	104.00
2	R	27	C	C2-N1-C1'	5.38	124.72	118.80
2	R	5	C	O4'-C1'-N1	-5.34	103.93	108.20
2	R	27	C	N3-C2-O2	-5.28	118.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	4	C	N1-C1'-C2'	5.27	120.85	114.00
2	R	42	C	N1-C1'-C2'	5.26	120.84	114.00
2	R	14	C	O4'-C1'-N1	5.24	112.39	108.20
2	R	18	C	C3'-C2'-C1'	5.22	105.68	101.50
2	R	42	C	C6-N1-C2	-5.20	118.22	120.30
2	R	30	C	N1-C1'-C2'	5.10	120.63	114.00
2	R	10	C	O4'-C1'-N1	-5.09	104.13	108.20
2	R	12	C	N1-C1'-C2'	5.08	120.61	114.00
2	R	10	C	C2-N1-C1'	5.08	124.39	118.80
2	R	33	C	C2-N1-C1'	5.07	124.38	118.80
2	R	40	C	OP2-P-O3'	-5.06	94.06	105.20
2	R	21	C	P-O3'-C3'	5.04	125.75	119.70
2	R	10	C	N3-C4-N4	5.04	121.53	118.00
2	R	40	C	N1-C1'-C2'	5.00	120.50	114.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	GLU	Peptide
1	A	78	LYS	Peptide
1	B	107	LEU	Peptide
1	B	167	ILE	Peptide
1	B	169	GLU	Peptide
1	B	170	GLN	Peptide
1	C	107	LEU	Peptide
1	D	107	LEU	Peptide
1	E	166	MET	Peptide
1	E	167	ILE	Peptide
1	E	169	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3327	0	3287	294	0
1	B	3290	0	3253	317	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3275	0	3242	319	0
1	D	3298	0	3264	293	0
1	E	3327	0	3287	288	0
2	R	900	0	496	82	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	R	5	0	0	0	0
All	All	17437	0	16829	1458	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 43.

All (1458) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:GLN:O	1:E:167:ILE:HB	1.36	1.25
1:B:317:ARG:HD3	2:R:22:C:O2'	1.41	1.18
1:E:177:GLU:HA	1:E:181:ILE:HD11	1.31	1.12
1:C:317:ARG:NH2	2:R:14:C:H5'	1.64	1.11
1:A:317:ARG:NH2	2:R:32:C:H5'	1.64	1.11
1:D:177:GLU:HA	1:D:181:ILE:HD11	1.32	1.10
1:C:177:GLU:HA	1:C:181:ILE:HD11	1.33	1.09
1:A:177:GLU:HA	1:A:181:ILE:HD11	1.33	1.09
1:B:60:LYS:O	1:B:61:SER:HB3	1.53	1.09
1:B:317:ARG:NH2	2:R:23:C:H5'	1.66	1.09
1:D:364:LEU:HD23	1:D:365:THR:H	1.16	1.09
1:E:169:GLU:HG2	1:E:170:GLN:H	1.15	1.06
1:B:168:ASN:O	1:B:169:GLU:HG2	1.53	1.05
1:B:177:GLU:HA	1:B:181:ILE:HD11	1.33	1.05
1:D:72:TYR:HE1	1:D:134:LEU:HD12	1.22	1.05
1:B:72:TYR:HE1	1:B:134:LEU:HD12	1.22	1.04
1:E:72:TYR:HE1	1:E:134:LEU:HD12	1.21	1.04
1:E:317:ARG:NH2	2:R:41:C:H5'	1.72	1.02
1:D:263:LEU:HD12	1:D:264:PRO:HD2	1.42	1.02
1:E:263:LEU:HD12	1:E:264:PRO:HD2	1.41	1.01
1:A:263:LEU:HD12	1:A:264:PRO:HD2	1.40	1.01
1:B:263:LEU:HD12	1:B:264:PRO:HD2	1.45	0.98
1:C:263:LEU:HD12	1:C:264:PRO:HD2	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:TYR:HE1	1:A:134:LEU:HD12	1.28	0.97
1:B:117:LEU:HB2	1:B:118:PRO:HD3	1.44	0.97
1:A:165:LYS:O	1:A:167:ILE:HD12	1.65	0.96
1:B:356:THR:HG23	1:B:357:PRO:HD3	1.46	0.96
1:C:356:THR:HG23	1:C:357:PRO:HD3	1.45	0.95
1:A:117:LEU:HB2	1:A:118:PRO:HD3	1.48	0.95
1:B:317:ARG:HD3	2:R:22:C:HO2'	1.32	0.95
1:C:72:TYR:HE1	1:C:134:LEU:HD12	1.28	0.94
1:D:356:THR:HG23	1:D:357:PRO:HD3	1.50	0.94
1:A:60:LYS:O	1:A:61:SER:HB3	1.68	0.93
1:A:356:THR:HG23	1:A:357:PRO:HD3	1.51	0.93
1:E:117:LEU:HB2	1:E:118:PRO:HD3	1.51	0.92
1:D:43:ASN:HA	1:D:111:LYS:HG3	1.48	0.92
1:B:43:ASN:HA	1:B:111:LYS:HG3	1.50	0.92
1:A:65:SER:HB2	1:A:117:LEU:HD11	1.50	0.91
1:C:317:ARG:HD3	2:R:13:C:O2'	1.68	0.91
1:D:65:SER:HB2	1:D:117:LEU:HD11	1.51	0.91
1:E:43:ASN:HA	1:E:111:LYS:HG3	1.51	0.91
1:E:356:THR:HG23	1:E:357:PRO:HD3	1.49	0.91
1:C:43:ASN:HA	1:C:111:LYS:HG3	1.49	0.91
1:C:117:LEU:HB2	1:C:118:PRO:HD3	1.50	0.91
1:E:60:LYS:O	1:E:61:SER:HB3	1.72	0.90
1:E:65:SER:HB2	1:E:117:LEU:HD11	1.50	0.90
1:B:150:PRO:HA	1:B:152:TYR:CE1	2.05	0.90
1:B:380:GLY:HA2	1:C:354:LYS:HZ3	1.37	0.90
1:A:43:ASN:HA	1:A:111:LYS:HG3	1.51	0.90
1:D:117:LEU:HB2	1:D:118:PRO:HD3	1.52	0.89
1:B:164:CYS:HA	1:B:168:ASN:HA	1.52	0.89
1:C:317:ARG:NE	1:C:317:ARG:H	1.70	0.89
1:D:354:LYS:HE3	1:D:356:THR:HA	1.55	0.89
1:A:150:PRO:HA	1:A:152:TYR:CE1	2.07	0.89
1:C:65:SER:HB2	1:C:117:LEU:HD11	1.51	0.89
1:C:150:PRO:HA	1:C:152:TYR:CE1	2.08	0.89
1:D:316:ALA:HA	1:D:317:ARG:NH2	1.88	0.89
1:E:354:LYS:HE3	1:E:356:THR:HA	1.55	0.89
1:B:317:ARG:CD	2:R:22:C:O2'	2.20	0.88
1:B:380:GLY:HA2	1:C:354:LYS:NZ	1.88	0.88
1:B:65:SER:HB2	1:B:117:LEU:HD11	1.52	0.88
1:E:317:ARG:HG3	2:R:40:C:N3	1.88	0.87
1:C:167:ILE:O	1:C:169:GLU:HG2	1.74	0.87
1:B:177:GLU:HG2	1:B:179:ARG:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ILE:HD12	1:D:74:TYR:HB2	1.55	0.87
1:A:42:ILE:HD12	1:A:74:TYR:HB2	1.57	0.86
1:D:150:PRO:HA	1:D:152:TYR:CE1	2.11	0.86
1:C:177:GLU:HG2	1:C:179:ARG:H	1.40	0.85
1:C:354:LYS:HE3	1:C:356:THR:HA	1.57	0.85
1:D:60:LYS:O	1:D:61:SER:HB3	1.73	0.85
1:E:169:GLU:HG2	1:E:170:GLN:N	1.86	0.85
1:A:177:GLU:HG2	1:A:179:ARG:H	1.41	0.84
1:B:168:ASN:C	1:B:169:GLU:HG2	1.93	0.84
1:B:354:LYS:HE3	1:B:356:THR:HA	1.59	0.84
1:C:376:VAL:HG13	1:D:354:LYS:HB2	1.57	0.84
1:E:165:LYS:O	1:E:167:ILE:HG13	1.76	0.84
1:B:42:ILE:HD12	1:B:74:TYR:HB2	1.57	0.84
1:D:72:TYR:CE1	1:D:134:LEU:HD12	2.12	0.84
1:E:150:PRO:HA	1:E:152:TYR:CE1	2.11	0.84
1:D:165:LYS:O	1:D:167:ILE:HD12	1.78	0.84
1:C:165:LYS:HG2	1:C:166:MET:HG3	1.58	0.84
1:E:163:GLN:O	1:E:167:ILE:CB	2.22	0.84
1:D:177:GLU:HG2	1:D:179:ARG:H	1.43	0.84
1:C:317:ARG:HH21	2:R:14:C:H5'	1.40	0.83
1:E:42:ILE:HD12	1:E:74:TYR:HB2	1.57	0.83
1:E:177:GLU:HG2	1:E:179:ARG:H	1.41	0.83
1:D:74:TYR:CE1	1:D:78:LYS:HD2	2.14	0.83
1:E:72:TYR:CE1	1:E:134:LEU:HD12	2.11	0.82
1:D:317:ARG:H	1:D:317:ARG:NE	1.77	0.82
1:E:37:GLU:HB2	1:E:108:VAL:HG11	1.61	0.82
1:B:317:ARG:H	1:B:317:ARG:NE	1.76	0.82
1:A:354:LYS:HE3	1:A:356:THR:HA	1.62	0.81
1:B:376:VAL:HG21	1:C:352:ASP:OD1	1.80	0.81
1:B:317:ARG:HH21	2:R:23:C:H5'	1.43	0.81
1:C:60:LYS:O	1:C:61:SER:HB3	1.78	0.81
1:B:2:SER:O	1:C:243:GLU:HG3	1.81	0.81
1:A:376:VAL:HG21	1:B:352:ASP:OD1	1.82	0.80
1:C:317:ARG:CD	2:R:13:C:O2'	2.29	0.80
1:A:316:ALA:HA	1:A:317:ARG:NH2	1.97	0.80
1:C:42:ILE:HD12	1:C:74:TYR:HB2	1.63	0.80
1:E:74:TYR:CE1	1:E:78:LYS:HD2	2.17	0.79
1:D:37:GLU:HB2	1:D:108:VAL:HG11	1.63	0.79
1:C:72:TYR:CE1	1:C:134:LEU:HD12	2.17	0.79
1:A:37:GLU:HB2	1:A:108:VAL:HG11	1.64	0.79
1:A:166:MET:H	1:E:184:VAL:HG11	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:TYR:CE1	1:B:78:LYS:HD2	2.18	0.78
1:D:364:LEU:HD23	1:D:365:THR:N	1.98	0.78
1:E:136:LEU:HD22	1:E:163:GLN:HE21	1.48	0.78
1:E:169:GLU:CG	1:E:170:GLN:H	1.95	0.78
1:B:72:TYR:CE1	1:B:134:LEU:HD12	2.12	0.78
1:C:37:GLU:HB2	1:C:108:VAL:HG11	1.64	0.78
1:A:126:ARG:HA	1:A:126:ARG:HH11	1.48	0.78
1:A:317:ARG:NE	1:A:317:ARG:H	1.80	0.78
1:C:136:LEU:HD22	1:C:163:GLN:HE21	1.47	0.78
1:B:54:TYR:CE1	1:B:118:PRO:HB2	2.19	0.78
1:A:74:TYR:CE1	1:A:78:LYS:HD2	2.19	0.78
1:D:214:ARG:HA	1:D:217:THR:HG22	1.65	0.78
1:A:389:PRO:HA	1:A:393:MET:HE1	1.66	0.78
1:B:133:TRP:HB3	1:B:167:ILE:HD13	1.64	0.77
1:E:126:ARG:HA	1:E:126:ARG:HH11	1.49	0.77
1:B:47:SER:HB3	1:B:50:ASP:HB2	1.67	0.77
1:B:316:ALA:HA	1:B:317:ARG:NH2	1.99	0.77
1:D:44:THR:HG22	1:D:46:LYS:HG2	1.67	0.77
2:R:21:C:H5”	2:R:21:C:H6	1.49	0.77
1:B:214:ARG:HA	1:B:217:THR:HG22	1.67	0.76
1:B:44:THR:HG22	1:B:46:LYS:HG2	1.68	0.76
1:C:74:TYR:CE1	1:C:78:LYS:HD2	2.20	0.76
1:B:349:CYS:SG	1:E:8:ILE:HG22	2.25	0.76
1:C:165:LYS:NZ	1:C:165:LYS:HB2	2.00	0.76
1:E:54:TYR:CE1	1:E:118:PRO:HB2	2.21	0.76
1:A:44:THR:HG23	1:A:46:LYS:HE2	1.68	0.75
1:D:317:ARG:H	1:D:317:ARG:CZ	1.98	0.75
1:A:317:ARG:HH21	2:R:32:C:H5’	1.48	0.75
1:A:214:ARG:HA	1:A:217:THR:HG22	1.68	0.75
1:D:54:TYR:CE1	1:D:118:PRO:HB2	2.21	0.75
1:E:389:PRO:HA	1:E:393:MET:HE1	1.68	0.75
1:E:214:ARG:HA	1:E:217:THR:HG22	1.68	0.75
1:A:54:TYR:CE1	1:A:118:PRO:HB2	2.22	0.75
1:B:37:GLU:HB2	1:B:108:VAL:HG11	1.67	0.75
1:A:47:SER:HB3	1:A:50:ASP:HB2	1.69	0.75
1:D:136:LEU:HD22	1:D:163:GLN:HE21	1.50	0.74
1:C:184:VAL:HG13	1:D:165:LYS:HG3	1.69	0.74
1:A:72:TYR:CE1	1:A:134:LEU:HD12	2.18	0.74
1:A:136:LEU:HD22	1:A:163:GLN:HE21	1.52	0.74
2:R:18:C:H2’	2:R:19:C:O4’	1.87	0.74
1:A:226:ALA:HB2	2:R:31:C:H5’	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:HA	1:C:217:THR:HG22	1.69	0.74
1:A:60:LYS:O	1:A:61:SER:CB	2.36	0.74
1:A:380:GLY:HA2	1:B:354:LYS:HZ3	1.52	0.74
1:C:44:THR:HG22	1:C:46:LYS:HG2	1.69	0.74
1:B:136:LEU:HD22	1:B:163:GLN:HE21	1.52	0.74
1:B:230:THR:HG21	1:B:298:HIS:CE1	2.23	0.73
1:B:383:GLU:HG3	1:C:354:LYS:HE2	1.71	0.73
1:D:126:ARG:HH11	1:D:126:ARG:HA	1.52	0.73
1:D:151:GLU:OE1	1:D:155:LYS:NZ	2.21	0.73
1:B:376:VAL:HG13	1:C:354:LYS:HB2	1.71	0.73
1:C:181:ILE:H	1:C:181:ILE:HD12	1.52	0.73
1:D:91:PHE:CZ	1:D:267:GLU:HG3	2.24	0.73
1:E:133:TRP:HB3	1:E:167:ILE:HD13	1.69	0.73
1:A:2:SER:O	1:B:243:GLU:HG3	1.88	0.73
1:B:171:PHE:CZ	1:B:173:PRO:HG2	2.24	0.73
1:A:167:ILE:HG22	1:A:169:GLU:HG2	1.71	0.73
1:D:364:LEU:HD22	1:D:368:ALA:HB2	1.70	0.73
1:B:126:ARG:HH11	1:B:126:ARG:HA	1.52	0.73
1:A:380:GLY:HA2	1:B:354:LYS:NZ	2.04	0.73
1:C:380:GLY:HA2	1:D:354:LYS:NZ	2.04	0.72
1:D:27:TYR:HB3	1:D:266:GLN:NE2	2.04	0.72
1:D:230:THR:HG21	1:D:298:HIS:CE1	2.24	0.72
1:E:317:ARG:H	1:E:317:ARG:NE	1.87	0.72
1:E:364:LEU:HB2	1:E:368:ALA:HB2	1.70	0.72
1:C:317:ARG:O	1:C:319:PRO:HD3	1.90	0.72
1:D:74:TYR:CD1	1:D:78:LYS:HD2	2.24	0.72
1:A:153:ARG:HH12	1:A:176:PRO:C	1.92	0.72
1:E:288:PRO:HG2	1:E:289:TYR:CE2	2.24	0.72
2:R:36:C:H2'	2:R:37:C:O4'	1.90	0.72
1:B:44:THR:HG23	1:B:46:LYS:HE2	1.71	0.72
1:D:29:ALA:HB2	1:D:91:PHE:CE2	2.25	0.72
1:D:42:ILE:CD1	1:D:74:TYR:HB2	2.18	0.72
1:E:44:THR:HG23	1:E:46:LYS:HE2	1.72	0.72
1:E:47:SER:HB3	1:E:50:ASP:HB2	1.71	0.72
1:E:60:LYS:O	1:E:61:SER:CB	2.37	0.72
1:C:126:ARG:HA	1:C:126:ARG:HH11	1.52	0.72
1:B:29:ALA:HB2	1:B:91:PHE:HE2	1.54	0.72
1:B:60:LYS:O	1:B:61:SER:CB	2.33	0.72
1:E:316:ALA:HA	1:E:317:ARG:NH2	2.04	0.72
1:B:184:VAL:HG11	1:C:166:MET:H	1.55	0.72
1:C:44:THR:HG23	1:C:46:LYS:HE2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ALA:HB2	1:D:91:PHE:HE2	1.54	0.72
1:D:44:THR:HG23	1:D:46:LYS:HE2	1.72	0.72
1:E:74:TYR:CD1	1:E:78:LYS:HD2	2.25	0.72
1:A:42:ILE:CD1	1:A:74:TYR:HB2	2.21	0.71
1:A:181:ILE:HD12	1:A:181:ILE:H	1.54	0.71
1:A:74:TYR:CD1	1:A:78:LYS:HD2	2.26	0.71
1:C:54:TYR:CE1	1:C:118:PRO:HB2	2.25	0.71
1:C:389:PRO:HA	1:C:393:MET:HE2	1.72	0.71
1:D:41:TYR:HE1	1:D:110:LEU:HD12	1.56	0.71
1:E:130:ASP:C	1:E:132:LYS:H	1.93	0.71
1:C:230:THR:HG21	1:C:298:HIS:CE1	2.26	0.71
1:D:47:SER:HB3	1:D:50:ASP:HB2	1.73	0.71
1:B:317:ARG:O	1:B:319:PRO:HD3	1.91	0.71
1:A:130:ASP:C	1:A:132:LYS:H	1.94	0.71
1:A:44:THR:HG22	1:A:46:LYS:HG2	1.72	0.70
1:A:105:PHE:C	1:A:107:LEU:H	1.95	0.70
1:C:316:ALA:HA	1:C:317:ARG:NH2	2.06	0.70
1:D:288:PRO:HG2	1:D:289:TYR:CE2	2.26	0.70
1:E:165:LYS:O	1:E:167:ILE:CG1	2.39	0.70
1:B:74:TYR:CD1	1:B:78:LYS:HD2	2.25	0.70
1:B:168:ASN:O	1:B:169:GLU:CG	2.36	0.70
1:C:47:SER:HB3	1:C:50:ASP:HB2	1.73	0.70
1:B:42:ILE:CD1	1:B:74:TYR:HB2	2.21	0.70
1:D:130:ASP:C	1:D:132:LYS:H	1.93	0.70
1:A:354:LYS:HB2	1:E:376:VAL:HG13	1.73	0.70
1:C:317:ARG:NE	2:R:13:C:O2'	2.24	0.70
1:A:168:ASN:O	1:A:169:GLU:OE2	2.09	0.70
1:E:44:THR:HG22	1:E:46:LYS:HG2	1.72	0.70
1:E:91:PHE:CZ	1:E:267:GLU:HG3	2.26	0.70
1:D:317:ARG:NH2	2:R:5:C:O5'	2.25	0.70
1:D:389:PRO:HA	1:D:393:MET:HE2	1.73	0.70
1:E:230:THR:HG21	1:E:298:HIS:CE1	2.26	0.70
1:E:45:THR:H	1:E:111:LYS:HZ1	1.38	0.70
1:B:398:LYS:HG2	1:B:402:MET:HE2	1.73	0.69
1:A:376:VAL:HG13	1:B:354:LYS:HB2	1.74	0.69
1:C:380:GLY:HA2	1:D:354:LYS:HZ3	1.56	0.69
1:A:317:ARG:O	1:A:319:PRO:HD3	1.92	0.69
1:E:42:ILE:CD1	1:E:74:TYR:HB2	2.22	0.69
1:B:171:PHE:CG	1:B:172:GLU:N	2.60	0.69
1:C:74:TYR:CD1	1:C:78:LYS:HD2	2.27	0.69
1:C:149:MET:O	1:C:151:GLU:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:ASP:OD1	1:D:214:ARG:HD2	1.93	0.69
1:A:167:ILE:HG22	1:A:169:GLU:CG	2.23	0.69
1:B:117:LEU:HB2	1:B:118:PRO:CD	2.22	0.69
1:B:130:ASP:C	1:B:132:LYS:H	1.95	0.69
1:B:253:GLU:H	1:B:253:GLU:CD	1.96	0.69
1:C:376:VAL:HG21	1:D:352:ASP:OD1	1.92	0.69
1:A:44:THR:CG2	1:A:46:LYS:HE2	2.23	0.69
1:A:91:PHE:CZ	1:A:267:GLU:HG3	2.27	0.69
1:C:29:ALA:HB2	1:C:91:PHE:HE2	1.57	0.69
1:C:130:ASP:C	1:C:132:LYS:H	1.95	0.69
1:E:153:ARG:HH12	1:E:176:PRO:C	1.96	0.69
1:D:253:GLU:H	1:D:253:GLU:CD	1.96	0.69
1:B:105:PHE:C	1:B:107:LEU:H	1.96	0.69
1:E:164:CYS:O	1:E:168:ASN:OD1	2.11	0.69
1:D:149:MET:O	1:D:151:GLU:N	2.26	0.68
1:B:173:PRO:C	1:B:174:LEU:HG	2.12	0.68
1:C:398:LYS:HG2	1:C:402:MET:HE3	1.74	0.68
1:A:165:LYS:HB2	1:A:165:LYS:NZ	2.08	0.68
1:A:230:THR:HG21	1:A:298:HIS:CE1	2.28	0.68
1:B:29:ALA:HB2	1:B:91:PHE:CE2	2.28	0.68
2:R:7:C:H4'	2:R:7:C:OP2	1.94	0.68
1:B:18:LEU:CD1	1:C:232:GLY:HA2	2.24	0.68
1:E:253:GLU:CD	1:E:253:GLU:H	1.97	0.68
1:B:97:LYS:O	1:B:100:ASP:HB2	1.92	0.68
1:B:181:ILE:HD12	1:B:181:ILE:H	1.59	0.68
1:C:288:PRO:HG2	1:C:289:TYR:CE2	2.28	0.68
1:D:173:PRO:C	1:D:174:LEU:HG	2.12	0.68
1:B:27:TYR:HB3	1:B:266:GLN:NE2	2.09	0.68
1:A:67:ILE:HD12	1:A:67:ILE:H	1.59	0.67
1:B:262:MET:HE2	1:B:262:MET:HA	1.75	0.67
1:D:45:THR:H	1:D:111:LYS:HZ1	1.40	0.67
1:B:91:PHE:CZ	1:B:267:GLU:HG3	2.28	0.67
1:C:317:ARG:H	1:C:317:ARG:CZ	2.06	0.67
1:E:25:VAL:HG11	1:E:288:PRO:HA	1.77	0.67
1:E:181:ILE:H	1:E:181:ILE:HD12	1.60	0.67
1:E:317:ARG:O	1:E:319:PRO:HD3	1.95	0.67
1:B:45:THR:H	1:B:111:LYS:HZ1	1.42	0.67
1:C:29:ALA:HB2	1:C:91:PHE:CE2	2.30	0.67
1:A:153:ARG:NH1	1:A:176:PRO:C	2.48	0.67
1:C:105:PHE:C	1:C:107:LEU:H	1.98	0.67
1:C:148:GLN:HG2	1:C:179:ARG:NH1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ARG:HH12	1:D:176:PRO:C	1.98	0.67
1:D:317:ARG:CZ	2:R:5:C:OP2	2.43	0.67
1:E:67:ILE:HD12	1:E:67:ILE:H	1.60	0.67
1:E:149:MET:O	1:E:151:GLU:N	2.28	0.67
1:A:97:LYS:O	1:A:100:ASP:HB2	1.95	0.67
1:E:41:TYR:HE1	1:E:110:LEU:HD12	1.59	0.67
1:A:7:ARG:NH1	1:B:259:VAL:HG21	2.09	0.66
1:A:199:ASP:OD1	1:A:214:ARG:HD2	1.95	0.66
1:D:262:MET:HE2	1:D:262:MET:HA	1.75	0.66
1:E:105:PHE:C	1:E:107:LEU:H	1.98	0.66
1:C:2:SER:O	1:D:243:GLU:HG3	1.95	0.66
1:E:173:PRO:C	1:E:174:LEU:HG	2.14	0.66
1:A:165:LYS:O	1:A:166:MET:HB2	1.95	0.66
1:B:117:LEU:CB	1:B:118:PRO:HD3	2.23	0.66
1:C:42:ILE:CD1	1:C:74:TYR:HB2	2.24	0.66
1:C:167:ILE:O	1:C:169:GLU:CG	2.42	0.66
1:A:151:GLU:OE1	1:A:155:LYS:NZ	2.29	0.66
1:B:107:LEU:N	1:B:107:LEU:HD12	2.10	0.66
1:B:199:ASP:OD1	1:B:214:ARG:HD2	1.95	0.66
1:C:173:PRO:C	1:C:174:LEU:HG	2.15	0.66
1:E:226:ALA:O	1:E:230:THR:HG23	1.96	0.66
1:A:253:GLU:CD	1:A:253:GLU:H	1.99	0.66
1:C:27:TYR:HB3	1:C:266:GLN:NE2	2.10	0.66
1:C:149:MET:C	1:C:151:GLU:H	1.99	0.66
1:D:81:ARG:CB	1:D:208:HIS:HE2	2.09	0.66
1:E:164:CYS:HA	1:E:168:ASN:HA	1.77	0.66
1:E:302:GLN:HG2	1:E:316:ALA:CB	2.26	0.66
1:A:27:TYR:HB3	1:A:266:GLN:NE2	2.11	0.65
1:E:199:ASP:OD1	1:E:214:ARG:HD2	1.96	0.65
1:B:18:LEU:HD12	1:C:232:GLY:HA2	1.78	0.65
1:A:302:GLN:HG2	1:A:316:ALA:CB	2.27	0.65
1:B:106:ASP:C	1:B:107:LEU:HD12	2.16	0.65
1:B:149:MET:O	1:B:151:GLU:N	2.30	0.65
1:C:151:GLU:OE1	1:C:155:LYS:NZ	2.29	0.65
1:C:376:VAL:HG13	1:D:354:LYS:CB	2.26	0.65
1:B:148:GLN:HG2	1:B:179:ARG:NH1	2.11	0.65
1:B:151:GLU:OE1	1:B:155:LYS:NZ	2.29	0.65
1:B:317:ARG:NE	1:B:317:ARG:N	2.44	0.65
1:C:317:ARG:NE	2:R:13:C:HO2'	1.95	0.65
1:D:181:ILE:HD12	1:D:181:ILE:H	1.62	0.65
1:A:117:LEU:HB2	1:A:118:PRO:CD	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PRO:C	1:A:174:LEU:HG	2.16	0.65
1:C:61:SER:O	1:C:63:ASN:N	2.30	0.65
1:D:97:LYS:O	1:D:100:ASP:HB2	1.97	0.65
1:D:149:MET:C	1:D:151:GLU:H	2.00	0.65
1:E:357:PRO:HA	1:E:360:SER:OG	1.96	0.65
1:A:226:ALA:HB2	2:R:31:C:C5'	2.26	0.65
1:B:67:ILE:HD12	1:B:67:ILE:H	1.62	0.65
1:C:41:TYR:HE1	1:C:110:LEU:HD12	1.61	0.65
1:B:317:ARG:H	1:B:317:ARG:CZ	2.10	0.64
1:D:61:SER:O	1:D:63:ASN:N	2.30	0.64
1:D:143:ARG:HH12	2:R:9:C:H5'	1.63	0.64
1:D:226:ALA:O	1:D:230:THR:HG23	1.98	0.64
1:E:44:THR:CG2	1:E:46:LYS:HE2	2.28	0.64
1:E:81:ARG:CB	1:E:208:HIS:HE2	2.11	0.64
1:A:29:ALA:HB2	1:A:91:PHE:HE2	1.62	0.64
1:A:263:LEU:CD1	1:A:264:PRO:HD2	2.23	0.64
1:C:153:ARG:HH12	1:C:176:PRO:C	2.00	0.64
1:B:81:ARG:CB	1:B:208:HIS:HE2	2.11	0.64
1:D:67:ILE:HD12	1:D:67:ILE:H	1.61	0.64
1:A:41:TYR:HE1	1:A:110:LEU:HD12	1.62	0.64
1:B:153:ARG:HH12	1:B:176:PRO:C	2.01	0.64
1:C:67:ILE:HD12	1:C:67:ILE:H	1.63	0.64
1:C:253:GLU:CD	1:C:253:GLU:H	2.01	0.64
1:E:262:MET:HE2	1:E:262:MET:HA	1.77	0.64
1:C:117:LEU:HB2	1:C:118:PRO:CD	2.27	0.64
1:D:364:LEU:CD2	1:D:365:THR:H	2.04	0.64
1:B:389:PRO:HA	1:B:393:MET:HE1	1.80	0.64
1:D:44:THR:CG2	1:D:46:LYS:HE2	2.27	0.64
1:E:214:ARG:HA	1:E:217:THR:CG2	2.28	0.64
1:B:44:THR:CG2	1:B:46:LYS:HE2	2.27	0.64
1:B:165:LYS:O	1:B:167:ILE:HD12	1.98	0.64
1:D:50:ASP:OD2	1:D:120:GLY:HA2	1.98	0.64
1:B:288:PRO:HG2	1:B:289:TYR:CE2	2.32	0.64
1:D:155:LYS:NZ	2:R:8:C:OP2	2.28	0.64
1:E:97:LYS:O	1:E:100:ASP:HB2	1.98	0.64
1:C:97:LYS:O	1:C:100:ASP:HB2	1.97	0.63
1:E:153:ARG:NH1	1:E:176:PRO:C	2.52	0.63
1:A:317:ARG:H	1:A:317:ARG:CZ	2.11	0.63
1:C:228:LEU:HB2	1:C:289:TYR:HB3	1.79	0.63
1:D:317:ARG:NH1	2:R:5:C:OP2	2.32	0.63
1:E:148:GLN:HG2	1:E:179:ARG:NH1	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASN:O	1:A:44:THR:C	2.36	0.63
1:C:165:LYS:O	1:C:166:MET:HB2	1.97	0.63
1:E:375:VAL:O	1:E:379:LEU:HB2	1.99	0.63
1:A:288:PRO:HG2	1:A:289:TYR:CE2	2.34	0.63
1:A:383:GLU:HG3	1:B:354:LYS:HE2	1.80	0.63
1:B:184:VAL:HG11	1:C:166:MET:N	2.13	0.63
1:D:117:LEU:CB	1:D:118:PRO:HD3	2.27	0.63
1:D:148:GLN:HG2	1:D:179:ARG:NH1	2.13	0.63
1:C:81:ARG:CB	1:C:208:HIS:HE2	2.11	0.63
1:C:117:LEU:CB	1:C:118:PRO:HD3	2.27	0.63
1:D:148:GLN:O	1:D:152:TYR:HE2	1.82	0.63
1:B:18:LEU:HD12	1:C:232:GLY:CA	2.29	0.63
1:B:50:ASP:OD2	1:B:120:GLY:HA2	1.98	0.63
1:D:31:TYR:C	1:D:31:TYR:CD1	2.71	0.63
1:A:317:ARG:HD3	2:R:31:C:H2'	1.80	0.63
1:B:89:SER:O	1:B:90:SER:HB2	1.99	0.63
1:D:29:ALA:O	1:D:31:TYR:N	2.30	0.63
1:B:31:TYR:CD1	1:B:31:TYR:C	2.71	0.63
1:D:105:PHE:C	1:D:107:LEU:H	2.02	0.63
1:E:43:ASN:O	1:E:44:THR:C	2.37	0.63
1:B:168:ASN:C	1:B:169:GLU:CG	2.65	0.62
1:C:44:THR:CG2	1:C:46:LYS:HE2	2.28	0.62
1:C:59:LEU:O	1:C:61:SER:N	2.29	0.62
1:D:214:ARG:HA	1:D:217:THR:CG2	2.29	0.62
1:E:149:MET:C	1:E:151:GLU:H	2.01	0.62
1:E:410:LYS:NZ	2:R:40:C:H42	1.98	0.62
1:A:89:SER:O	1:A:90:SER:HB2	1.99	0.62
1:C:42:ILE:HD12	1:C:74:TYR:HD2	1.62	0.62
1:C:302:GLN:HG2	1:C:316:ALA:CB	2.30	0.62
1:A:127:THR:HG23	1:A:129:ALA:H	1.64	0.62
1:B:25:VAL:HG11	1:B:288:PRO:HA	1.82	0.62
1:B:43:ASN:O	1:B:44:THR:C	2.38	0.62
1:B:149:MET:C	1:B:151:GLU:H	2.02	0.62
1:B:375:VAL:O	1:B:379:LEU:HB2	1.97	0.62
1:B:380:GLY:CA	1:C:354:LYS:HZ3	2.12	0.62
1:C:31:TYR:CD1	1:C:31:TYR:C	2.72	0.62
1:A:228:LEU:HB2	1:A:289:TYR:HB3	1.82	0.62
1:A:117:LEU:CB	1:A:118:PRO:HD3	2.26	0.62
1:D:127:THR:HG23	1:D:129:ALA:H	1.64	0.62
1:E:133:TRP:CB	1:E:167:ILE:HD13	2.29	0.62
1:B:352:ASP:OD1	1:B:352:ASP:C	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PHE:CZ	1:C:267:GLU:HG3	2.34	0.62
1:D:153:ARG:NH1	1:D:176:PRO:C	2.54	0.62
1:D:302:GLN:HG2	1:D:316:ALA:CB	2.30	0.62
1:E:27:TYR:HB3	1:E:266:GLN:NE2	2.14	0.62
1:B:263:LEU:CD1	1:B:264:PRO:HD2	2.27	0.62
1:E:117:LEU:HB2	1:E:118:PRO:CD	2.27	0.62
1:D:263:LEU:CD1	1:D:264:PRO:HD2	2.25	0.61
1:A:375:VAL:O	1:A:379:LEU:HB2	2.00	0.61
1:B:150:PRO:CA	1:B:152:TYR:CE1	2.79	0.61
1:E:317:ARG:NH2	2:R:41:C:C5'	2.58	0.61
1:D:375:VAL:O	1:D:379:LEU:HB2	2.00	0.61
1:A:226:ALA:O	1:A:230:THR:HG23	2.00	0.61
1:C:45:THR:H	1:C:111:LYS:HZ1	1.46	0.61
1:B:184:VAL:HG13	1:C:165:LYS:HG3	1.82	0.61
1:C:165:LYS:HB2	1:C:165:LYS:HZ2	1.64	0.61
1:C:199:ASP:OD1	1:C:214:ARG:HD2	1.99	0.61
1:E:89:SER:O	1:E:90:SER:HB2	2.00	0.61
1:A:107:LEU:N	1:A:107:LEU:HD12	2.15	0.61
1:B:224:ASP:CG	2:R:21:C:H4'	2.20	0.61
1:E:398:LYS:HG2	1:E:402:MET:HE3	1.83	0.61
1:C:29:ALA:O	1:C:31:TYR:N	2.30	0.61
1:C:323:GLU:OE1	1:D:239:GLY:HA3	2.01	0.61
1:A:317:ARG:HH22	2:R:32:C:H5'	1.61	0.61
1:C:352:ASP:OD1	1:C:352:ASP:C	2.38	0.61
1:D:117:LEU:HB2	1:D:118:PRO:CD	2.28	0.61
1:D:228:LEU:HB2	1:D:289:TYR:HB3	1.80	0.61
1:A:149:MET:C	1:A:151:GLU:H	2.04	0.61
1:A:25:VAL:HG11	1:A:288:PRO:HA	1.83	0.61
1:A:214:ARG:HA	1:A:217:THR:CG2	2.31	0.61
1:A:259:VAL:HG21	1:E:7:ARG:NH1	2.16	0.61
1:B:29:ALA:O	1:B:31:TYR:N	2.30	0.61
1:B:214:ARG:HA	1:B:217:THR:CG2	2.30	0.61
1:A:31:TYR:CD1	1:A:31:TYR:C	2.73	0.60
1:A:150:PRO:CA	1:A:152:TYR:CE1	2.81	0.60
1:B:41:TYR:HE1	1:B:110:LEU:HD12	1.66	0.60
1:B:66:ILE:O	1:B:69:VAL:HG13	2.00	0.60
1:C:199:ASP:HB2	1:C:217:THR:HG23	1.83	0.60
1:D:43:ASN:O	1:D:44:THR:C	2.38	0.60
1:E:263:LEU:CD1	1:E:264:PRO:HD2	2.23	0.60
1:A:398:LYS:HG2	1:A:402:MET:HE2	1.83	0.60
1:C:45:THR:C	1:C:46:LYS:HD3	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LEU:HD12	1:C:107:LEU:N	2.16	0.60
1:A:81:ARG:CB	1:A:208:HIS:HE2	2.14	0.60
1:E:151:GLU:OE1	1:E:155:LYS:NZ	2.35	0.60
1:B:153:ARG:NH1	1:B:176:PRO:C	2.55	0.60
1:B:302:GLN:HG2	1:B:316:ALA:CB	2.31	0.60
1:C:25:VAL:HG11	1:C:288:PRO:HA	1.84	0.60
1:C:153:ARG:NH1	1:C:176:PRO:C	2.54	0.60
1:D:89:SER:O	1:D:90:SER:HB2	2.00	0.60
1:A:149:MET:O	1:A:151:GLU:N	2.34	0.60
1:B:150:PRO:HA	1:B:152:TYR:CD1	2.36	0.60
1:E:317:ARG:H	1:E:317:ARG:CZ	2.14	0.60
1:A:148:GLN:O	1:A:152:TYR:HE2	1.85	0.60
1:A:344:LEU:HD13	1:E:250:LEU:HB3	1.83	0.60
1:B:184:VAL:HG13	1:C:165:LYS:HA	1.84	0.60
1:C:180:ASP:OD2	1:D:164:CYS:HB3	2.00	0.60
1:C:317:ARG:NE	1:C:317:ARG:N	2.45	0.60
1:A:66:ILE:O	1:A:69:VAL:HG13	2.01	0.60
1:E:31:TYR:CD1	1:E:31:TYR:C	2.75	0.60
1:E:87:ASP:OD2	1:E:97:LYS:HG3	2.01	0.60
2:R:11:C:H2'	2:R:12:C:O4'	2.02	0.60
1:A:29:ALA:O	1:A:31:TYR:N	2.30	0.59
1:B:165:LYS:HB2	1:B:165:LYS:NZ	2.17	0.59
1:E:66:ILE:O	1:E:69:VAL:HG13	2.02	0.59
1:E:165:LYS:O	1:E:166:MET:HB2	2.01	0.59
2:R:12:C:C2'	2:R:13:C:H5'	2.31	0.59
1:B:228:LEU:HB2	1:B:289:TYR:HB3	1.84	0.59
1:D:352:ASP:OD1	1:D:352:ASP:C	2.40	0.59
1:A:148:GLN:HG2	1:A:179:ARG:NH1	2.16	0.59
1:C:42:ILE:HD12	1:C:74:TYR:CD2	2.36	0.59
1:E:117:LEU:CB	1:E:118:PRO:HD3	2.27	0.59
1:E:127:THR:HG23	1:E:129:ALA:H	1.66	0.59
1:B:383:GLU:HG3	1:C:354:LYS:CE	2.31	0.59
1:A:87:ASP:OD2	1:A:97:LYS:HG3	2.03	0.59
1:A:262:MET:HA	1:A:262:MET:HE2	1.84	0.59
1:D:317:ARG:O	1:D:319:PRO:HD3	2.02	0.59
1:C:214:ARG:HA	1:C:217:THR:CG2	2.32	0.59
1:C:263:LEU:CD1	1:C:264:PRO:HD2	2.27	0.59
1:D:15:VAL:O	1:D:17:LYS:HG2	2.03	0.59
1:A:169:GLU:HA	1:A:170:GLN:NE2	2.17	0.59
1:B:226:ALA:O	1:B:230:THR:HG23	2.02	0.59
1:E:228:LEU:HB2	1:E:289:TYR:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:VAL:HG11	1:D:288:PRO:HA	1.85	0.58
1:A:352:ASP:OD1	1:A:352:ASP:C	2.42	0.58
1:D:66:ILE:O	1:D:69:VAL:HG13	2.03	0.58
1:B:22:GLU:HB3	1:C:206:LYS:NZ	2.18	0.58
1:C:50:ASP:OD2	1:C:120:GLY:HA2	2.03	0.58
1:C:262:MET:HA	1:C:262:MET:HE2	1.84	0.58
1:A:152:TYR:HD1	1:A:153:ARG:H	1.51	0.58
1:B:148:GLN:O	1:B:152:TYR:HE2	1.87	0.58
2:R:25:C:H2'	2:R:26:C:C6	2.38	0.58
1:A:106:ASP:C	1:A:107:LEU:HD12	2.23	0.58
1:C:375:VAL:O	1:C:379:LEU:HB2	2.03	0.58
1:D:152:TYR:HD1	1:D:153:ARG:H	1.52	0.58
1:B:68:HIS:HE1	1:B:117:LEU:HG	1.67	0.58
1:D:412:ILE:C	1:D:412:ILE:HD12	2.24	0.58
1:A:317:ARG:NE	1:A:317:ARG:N	2.50	0.58
1:B:22:GLU:HB3	1:C:206:LYS:HZ3	1.68	0.58
1:B:81:ARG:HB2	1:B:208:HIS:HE2	1.68	0.58
1:D:29:ALA:C	1:D:31:TYR:H	2.07	0.58
1:A:389:PRO:HA	1:A:393:MET:CE	2.34	0.58
1:B:29:ALA:C	1:B:31:TYR:H	2.08	0.58
1:C:226:ALA:O	1:C:230:THR:HG23	2.04	0.58
1:B:127:THR:HG23	1:B:129:ALA:H	1.69	0.58
1:A:150:PRO:HA	1:A:152:TYR:CD1	2.38	0.57
1:C:150:PRO:CA	1:C:152:TYR:CE1	2.83	0.57
1:D:107:LEU:N	1:D:107:LEU:HD12	2.19	0.57
1:A:130:ASP:O	1:A:132:LYS:N	2.36	0.57
1:B:87:ASP:OD2	1:B:97:LYS:HG3	2.05	0.57
1:C:66:ILE:O	1:C:69:VAL:HG13	2.04	0.57
1:C:152:TYR:HD1	1:C:153:ARG:H	1.52	0.57
1:E:130:ASP:O	1:E:132:LYS:N	2.36	0.57
1:A:14:ILE:HG23	1:A:16:PRO:HD3	1.87	0.57
1:A:165:LYS:NZ	1:A:165:LYS:CB	2.67	0.57
1:C:180:ASP:OD2	1:C:180:ASP:C	2.43	0.57
1:D:317:ARG:NE	1:D:317:ARG:N	2.48	0.57
1:C:165:LYS:O	1:C:166:MET:CB	2.53	0.57
1:D:87:ASP:OD2	1:D:97:LYS:HG3	2.05	0.57
1:D:178:GLY:O	1:D:179:ARG:HB2	2.05	0.57
1:E:50:ASP:OD2	1:E:120:GLY:HA2	2.05	0.57
1:E:165:LYS:HB2	1:E:165:LYS:NZ	2.18	0.57
1:E:224:ASP:CG	2:R:39:C:H4'	2.25	0.57
1:A:29:ALA:HB2	1:A:91:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ILE:HD11	1:D:259:VAL:HA	1.86	0.57
1:C:294:ASN:N	1:C:295:PRO:HD3	2.20	0.57
1:C:14:ILE:HG23	1:C:16:PRO:HD3	1.87	0.57
1:C:106:ASP:C	1:C:107:LEU:HD12	2.25	0.57
1:C:342:ALA:HB1	1:C:344:LEU:HD23	1.87	0.57
1:C:383:GLU:HG3	1:D:354:LYS:HE2	1.86	0.57
1:E:199:ASP:HB2	1:E:217:THR:HG23	1.86	0.57
2:R:21:C:C2'	2:R:22:C:H5'	2.35	0.57
1:A:70:ASN:N	1:A:70:ASN:HD22	2.03	0.57
1:A:117:LEU:HD23	1:A:117:LEU:N	2.20	0.57
1:B:152:TYR:HD1	1:B:153:ARG:H	1.53	0.57
1:C:292:VAL:HG12	2:R:13:C:H5	1.70	0.57
1:A:323:GLU:OE1	1:B:239:GLY:HA3	2.05	0.57
1:C:46:LYS:HD3	1:C:46:LYS:N	2.19	0.57
1:C:171:PHE:CG	1:C:172:GLU:N	2.72	0.57
1:D:143:ARG:NH1	2:R:9:C:H5'	2.20	0.57
1:D:171:PHE:CG	1:D:172:GLU:N	2.73	0.57
1:E:262:MET:HA	1:E:262:MET:CE	2.35	0.57
1:D:27:TYR:HB3	1:D:266:GLN:HE22	1.68	0.56
1:D:215:TYR:HA	2:R:9:C:O4'	2.04	0.56
1:A:199:ASP:OD1	1:A:217:THR:HG23	2.05	0.56
1:B:262:MET:HA	1:B:262:MET:CE	2.35	0.56
1:C:150:PRO:HA	1:C:152:TYR:CD1	2.40	0.56
1:C:165:LYS:NZ	1:C:165:LYS:CB	2.67	0.56
1:D:70:ASN:N	1:D:70:ASN:HD22	2.04	0.56
1:D:106:ASP:C	1:D:107:LEU:HD12	2.26	0.56
1:E:152:TYR:HD1	1:E:153:ARG:H	1.53	0.56
1:D:81:ARG:HB2	1:D:208:HIS:HE2	1.70	0.56
1:A:171:PHE:CG	1:A:172:GLU:N	2.73	0.56
1:A:199:ASP:HB2	1:A:217:THR:HG23	1.87	0.56
1:B:133:TRP:CB	1:B:167:ILE:HD13	2.34	0.56
1:C:89:SER:O	1:C:90:SER:HB2	2.05	0.56
1:C:43:ASN:O	1:C:44:THR:C	2.43	0.56
1:C:68:HIS:HE1	1:C:117:LEU:HG	1.70	0.56
1:C:117:LEU:N	1:C:117:LEU:HD23	2.21	0.56
1:D:214:ARG:CA	1:D:217:THR:HG22	2.35	0.56
1:C:199:ASP:CB	1:C:217:THR:HG23	2.36	0.56
1:E:58:GLY:O	1:E:63:ASN:O	2.24	0.56
1:B:45:THR:C	1:B:46:LYS:HD3	2.26	0.56
1:D:148:GLN:O	1:D:152:TYR:CE2	2.59	0.56
2:R:40:C:H2'	2:R:40:C:O2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ILE:HD12	1:B:74:TYR:HD2	1.70	0.55
1:D:143:ARG:HH12	2:R:9:C:C5'	2.19	0.55
1:E:107:LEU:HD12	1:E:107:LEU:N	2.21	0.55
1:A:42:ILE:HD12	1:A:74:TYR:HD2	1.72	0.55
1:D:150:PRO:CA	1:D:152:TYR:CE1	2.86	0.55
1:A:165:LYS:O	1:A:167:ILE:CD1	2.48	0.55
1:C:29:ALA:C	1:C:31:TYR:H	2.08	0.55
1:D:68:HIS:HE1	1:D:117:LEU:HG	1.71	0.55
1:A:68:HIS:HE1	1:A:117:LEU:HG	1.70	0.55
1:B:163:GLN:O	1:B:167:ILE:HD12	2.05	0.55
1:B:178:GLY:O	1:B:179:ARG:HB2	2.05	0.55
1:C:127:THR:HG23	1:C:129:ALA:H	1.70	0.55
1:D:45:THR:C	1:D:46:LYS:HD3	2.27	0.55
1:E:29:ALA:O	1:E:31:TYR:N	2.33	0.55
1:C:167:ILE:O	1:C:168:ASN:C	2.44	0.55
1:D:136:LEU:C	1:D:136:LEU:HD23	2.27	0.55
1:E:150:PRO:CA	1:E:152:TYR:CE1	2.87	0.55
1:A:199:ASP:CB	1:A:217:THR:HG23	2.36	0.55
1:C:36:LYS:HG3	1:C:93:ILE:HD11	1.89	0.55
1:D:166:MET:C	1:D:167:ILE:HG13	2.25	0.55
1:D:224:ASP:CG	2:R:3:C:H4'	2.27	0.55
1:D:262:MET:HA	1:D:262:MET:CE	2.36	0.55
1:E:148:GLN:O	1:E:152:TYR:HE2	1.90	0.55
1:E:178:GLY:O	1:E:179:ARG:HB2	2.06	0.55
1:E:14:ILE:HG23	1:E:16:PRO:HD3	1.89	0.55
1:E:389:PRO:HA	1:E:393:MET:CE	2.37	0.55
1:D:165:LYS:HB2	1:D:165:LYS:NZ	2.22	0.55
1:E:68:HIS:HE1	1:E:117:LEU:HG	1.70	0.55
1:A:58:GLY:O	1:A:63:ASN:O	2.24	0.55
1:B:15:VAL:O	1:B:17:LYS:HG2	2.07	0.55
1:B:42:ILE:HD12	1:B:74:TYR:CD2	2.42	0.55
1:B:171:PHE:HZ	1:B:173:PRO:HG2	1.72	0.55
1:B:117:LEU:N	1:B:117:LEU:HD23	2.21	0.54
1:B:350:VAL:HG13	1:E:4:THR:O	2.07	0.54
2:R:16:C:H2'	2:R:17:C:C6	2.42	0.54
1:A:166:MET:H	1:E:184:VAL:CG1	2.18	0.54
1:A:167:ILE:HG22	1:A:169:GLU:OE1	2.07	0.54
1:A:214:ARG:CA	1:A:217:THR:HG22	2.37	0.54
1:B:365:THR:HG23	1:B:366:THR:H	1.72	0.54
1:A:180:ASP:OD2	1:A:180:ASP:C	2.44	0.54
1:A:385:GLN:HG2	1:A:390:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:HIS:O	1:B:206:LYS:HG3	2.07	0.54
1:B:385:GLN:HG2	1:B:390:THR:HG22	1.89	0.54
1:C:70:ASN:N	1:C:70:ASN:HD22	2.05	0.54
1:C:385:GLN:HG2	1:C:390:THR:HG22	1.90	0.54
1:E:294:ASN:N	1:E:295:PRO:HD3	2.22	0.54
1:B:43:ASN:OD1	1:B:112:ALA:N	2.41	0.54
1:B:81:ARG:HD2	1:B:208:HIS:HE2	1.73	0.54
1:C:167:ILE:O	1:C:169:GLU:CD	2.46	0.54
1:D:42:ILE:HD12	1:D:74:TYR:HD2	1.73	0.54
1:D:70:ASN:HD22	1:D:70:ASN:H	1.55	0.54
1:D:398:LYS:HG2	1:D:402:MET:HE2	1.90	0.54
1:E:29:ALA:C	1:E:31:TYR:H	2.11	0.54
1:E:214:ARG:CA	1:E:217:THR:HG22	2.37	0.54
1:A:153:ARG:NH1	1:A:176:PRO:O	2.39	0.54
1:D:42:ILE:HD12	1:D:74:TYR:CD2	2.43	0.54
1:D:130:ASP:O	1:D:132:LYS:N	2.36	0.54
1:D:385:GLN:HG2	1:D:390:THR:HG22	1.90	0.54
2:R:12:C:H2'	2:R:13:C:H5'	1.89	0.54
1:C:43:ASN:OD1	1:C:112:ALA:N	2.41	0.54
1:C:203:HIS:O	1:C:206:LYS:HG3	2.08	0.54
1:D:150:PRO:HA	1:D:152:TYR:CD1	2.41	0.54
1:D:203:HIS:O	1:D:206:LYS:HG3	2.07	0.54
1:E:70:ASN:HD22	1:E:70:ASN:N	2.05	0.54
1:A:42:ILE:HD12	1:A:74:TYR:CD2	2.43	0.54
1:B:130:ASP:O	1:B:132:LYS:N	2.39	0.54
1:B:295:PRO:HB2	1:B:322:ILE:CG2	2.38	0.54
1:C:178:GLY:O	1:C:179:ARG:HB2	2.08	0.54
1:E:42:ILE:HD12	1:E:74:TYR:HD2	1.73	0.54
1:E:171:PHE:CG	1:E:172:GLU:N	2.74	0.54
1:B:150:PRO:HD3	1:B:152:TYR:OH	2.08	0.54
1:C:130:ASP:O	1:C:132:LYS:N	2.38	0.54
1:C:203:HIS:HD2	1:C:272:ASP:OD1	1.89	0.54
1:E:106:ASP:C	1:E:107:LEU:HD12	2.28	0.54
1:A:243:GLU:HG3	1:E:2:SER:O	2.08	0.54
1:B:214:ARG:CA	1:B:217:THR:HG22	2.38	0.54
1:C:309:ARG:N	1:C:309:ARG:HD2	2.23	0.54
1:E:167:ILE:HG22	1:E:168:ASN:N	2.22	0.54
1:E:352:ASP:C	1:E:352:ASP:OD1	2.46	0.54
1:E:359:ASP:O	1:E:361:THR:HG23	2.07	0.54
1:E:412:ILE:C	1:E:412:ILE:HD12	2.27	0.54
1:B:5:VAL:CG1	1:D:348:PHE:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ASP:OD2	1:C:97:LYS:HG3	2.08	0.54
1:C:308:LEU:O	1:C:309:ARG:HB2	2.08	0.54
1:A:50:ASP:OD2	1:A:120:GLY:HA2	2.08	0.53
1:B:46:LYS:HD3	1:B:46:LYS:N	2.21	0.53
1:C:385:GLN:O	1:C:386:ASN:HB2	2.08	0.53
1:E:81:ARG:HB2	1:E:208:HIS:HE2	1.72	0.53
1:A:323:GLU:O	1:A:327:LEU:HD22	2.08	0.53
1:D:147:THR:HG21	1:D:152:TYR:HB3	1.89	0.53
1:A:165:LYS:HB2	1:A:165:LYS:HZ2	1.71	0.53
1:B:136:LEU:C	1:B:136:LEU:HD23	2.28	0.53
1:B:389:PRO:HA	1:B:393:MET:CE	2.38	0.53
1:A:294:ASN:N	1:A:295:PRO:HD3	2.23	0.53
1:C:148:GLN:O	1:C:152:TYR:HE2	1.91	0.53
1:D:60:LYS:O	1:D:61:SER:CB	2.46	0.53
1:E:308:LEU:O	1:E:309:ARG:HB2	2.09	0.53
1:B:70:ASN:N	1:B:70:ASN:HD22	2.07	0.53
1:C:38:ILE:HD11	1:C:107:LEU:O	2.09	0.53
1:E:385:GLN:HG2	1:E:390:THR:HG22	1.89	0.53
1:D:309:ARG:HD2	1:D:309:ARG:N	2.24	0.53
1:E:323:GLU:O	1:E:327:LEU:HD22	2.09	0.53
1:C:172:GLU:HB3	1:C:173:PRO:CD	2.39	0.53
1:C:389:PRO:HA	1:C:393:MET:CE	2.37	0.53
1:E:149:MET:C	1:E:151:GLU:N	2.62	0.53
1:E:166:MET:HB2	1:E:167:ILE:HG13	1.89	0.53
1:A:370:PRO:HD3	1:A:381:TRP:CG	2.44	0.53
1:E:150:PRO:HA	1:E:152:TYR:CD1	2.43	0.53
1:A:203:HIS:HD2	1:A:272:ASP:OD1	1.91	0.53
1:B:27:TYR:HB3	1:B:266:GLN:HE22	1.73	0.53
1:B:294:ASN:N	1:B:295:PRO:HD3	2.24	0.53
1:D:117:LEU:HD23	1:D:117:LEU:N	2.24	0.53
1:B:230:THR:HG21	1:B:298:HIS:ND1	2.22	0.53
1:E:45:THR:H	1:E:111:LYS:NZ	2.07	0.53
1:E:199:ASP:CB	1:E:217:THR:HG23	2.38	0.53
1:A:203:HIS:O	1:A:206:LYS:HG3	2.09	0.52
1:D:81:ARG:HD2	1:D:208:HIS:HE2	1.74	0.52
1:E:45:THR:C	1:E:46:LYS:HD3	2.29	0.52
1:B:45:THR:H	1:B:111:LYS:NZ	2.06	0.52
1:E:104:ILE:O	1:E:107:LEU:HD13	2.10	0.52
1:A:398:LYS:HG2	1:A:402:MET:CE	2.39	0.52
1:D:230:THR:HG21	1:D:298:HIS:ND1	2.24	0.52
1:D:203:HIS:HD2	1:D:272:ASP:OD1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:HIS:O	1:E:206:LYS:HG3	2.09	0.52
1:E:230:THR:HG21	1:E:298:HIS:ND1	2.24	0.52
1:A:130:ASP:C	1:A:132:LYS:N	2.63	0.52
1:A:402:MET:SD	1:E:422:LYS:HD2	2.49	0.52
1:B:54:TYR:CD1	1:B:122:SER:HB2	2.45	0.52
1:B:308:LEU:O	1:B:309:ARG:HB2	2.08	0.52
1:C:165:LYS:O	1:C:167:ILE:HG12	2.08	0.52
1:D:308:LEU:O	1:D:309:ARG:HB2	2.10	0.52
1:B:31:TYR:C	1:B:33:ARG:H	2.12	0.52
1:B:223:LYS:O	1:B:224:ASP:HB2	2.09	0.52
1:C:31:TYR:C	1:C:33:ARG:H	2.13	0.52
1:C:136:LEU:C	1:C:136:LEU:HD23	2.29	0.52
1:D:149:MET:C	1:D:151:GLU:N	2.62	0.52
1:D:253:GLU:OE2	1:D:253:GLU:N	2.41	0.52
1:E:169:GLU:CG	1:E:170:GLN:N	2.60	0.52
2:R:27:C:C2'	2:R:28:C:O5'	2.58	0.52
1:A:31:TYR:C	1:A:33:ARG:H	2.13	0.52
1:A:43:ASN:OD1	1:A:112:ALA:N	2.42	0.52
1:A:298:HIS:NE2	1:A:317:ARG:NH1	2.58	0.52
1:A:309:ARG:N	1:A:309:ARG:HD2	2.25	0.52
1:C:151:GLU:O	1:C:155:LYS:HB2	2.09	0.52
1:D:294:ASN:N	1:D:295:PRO:HD3	2.25	0.52
1:E:163:GLN:O	1:E:167:ILE:HD12	2.10	0.52
1:A:178:GLY:O	1:A:179:ARG:HB2	2.08	0.51
1:B:253:GLU:OE2	1:B:253:GLU:N	2.39	0.51
1:B:370:PRO:HD3	1:B:381:TRP:CG	2.45	0.51
1:D:370:PRO:HD3	1:D:381:TRP:CG	2.45	0.51
1:D:389:PRO:HA	1:D:393:MET:CE	2.40	0.51
1:B:309:ARG:HD2	1:B:309:ARG:N	2.25	0.51
1:C:45:THR:H	1:C:111:LYS:NZ	2.07	0.51
1:C:342:ALA:CB	1:C:344:LEU:HD23	2.39	0.51
1:D:59:LEU:O	1:D:61:SER:N	2.42	0.51
1:E:36:LYS:HG3	1:E:93:ILE:HD11	1.92	0.51
1:E:54:TYR:CD1	1:E:122:SER:HB2	2.46	0.51
1:E:130:ASP:C	1:E:132:LYS:N	2.62	0.51
1:E:317:ARG:NE	1:E:317:ARG:N	2.56	0.51
1:C:81:ARG:HD2	1:C:208:HIS:HE2	1.74	0.51
1:D:180:ASP:OD2	1:D:180:ASP:C	2.48	0.51
1:A:149:MET:O	1:A:152:TYR:CD2	2.64	0.51
1:B:149:MET:C	1:B:151:GLU:N	2.64	0.51
1:B:298:HIS:NE2	1:B:317:ARG:NH1	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:PRO:HD3	1:C:381:TRP:CG	2.45	0.51
1:D:54:TYR:CD1	1:D:122:SER:HB2	2.46	0.51
1:E:59:LEU:HB3	1:E:172:GLU:HG2	1.93	0.51
1:E:61:SER:O	1:E:63:ASN:N	2.38	0.51
1:A:81:ARG:HD2	1:A:208:HIS:HE2	1.76	0.51
1:A:148:GLN:O	1:A:152:TYR:CE2	2.62	0.51
1:B:72:TYR:CD2	1:B:72:TYR:O	2.63	0.51
1:B:398:LYS:HG2	1:B:402:MET:CE	2.41	0.51
1:C:72:TYR:O	1:C:72:TYR:CD2	2.63	0.51
1:C:81:ARG:HB2	1:C:208:HIS:HE2	1.72	0.51
1:E:295:PRO:HB2	1:E:322:ILE:CG2	2.40	0.51
2:R:27:C:H2'	2:R:28:C:O5'	2.11	0.51
1:B:14:ILE:HG23	1:B:16:PRO:HD3	1.93	0.51
1:C:27:TYR:HB3	1:C:266:GLN:HE22	1.74	0.51
1:C:54:TYR:CD1	1:C:122:SER:HB2	2.45	0.51
1:C:184:VAL:HG13	1:D:165:LYS:CG	2.40	0.51
1:E:81:ARG:HD2	1:E:208:HIS:HE2	1.74	0.51
1:E:298:HIS:NE2	1:E:317:ARG:NH1	2.59	0.51
1:A:308:LEU:O	1:A:309:ARG:HB2	2.10	0.51
1:B:149:MET:C	1:B:152:TYR:CE2	2.84	0.51
1:B:171:PHE:HE2	1:B:173:PRO:O	1.94	0.51
1:C:149:MET:HB3	1:C:150:PRO:HD2	1.92	0.51
1:D:147:THR:CG2	1:D:152:TYR:HB3	2.41	0.51
1:D:408:ARG:NH2	2:R:6:C:H2'	2.26	0.51
1:E:309:ARG:HD2	1:E:309:ARG:N	2.26	0.51
1:A:342:ALA:HB1	1:A:344:LEU:HD23	1.93	0.51
1:C:147:THR:HG21	1:C:152:TYR:HB3	1.92	0.51
1:C:199:ASP:OD1	1:C:217:THR:HG23	2.10	0.51
1:C:214:ARG:CA	1:C:217:THR:HG22	2.40	0.51
1:A:136:LEU:HD23	1:A:136:LEU:C	2.32	0.51
1:B:171:PHE:CE2	1:B:173:PRO:O	2.64	0.51
1:C:323:GLU:O	1:C:327:LEU:HD22	2.10	0.51
1:D:72:TYR:CD2	1:D:72:TYR:C	2.82	0.51
1:D:130:ASP:C	1:D:132:LYS:N	2.62	0.51
1:D:199:ASP:HB2	1:D:217:THR:HG23	1.91	0.51
1:E:15:VAL:O	1:E:17:LYS:HG2	2.11	0.51
1:E:151:GLU:O	1:E:155:LYS:HB2	2.10	0.51
1:A:45:THR:C	1:A:46:LYS:HD3	2.30	0.51
1:A:54:TYR:CD1	1:A:122:SER:HB2	2.46	0.51
1:A:383:GLU:HG3	1:B:354:LYS:CE	2.41	0.51
1:D:401:VAL:HG21	1:D:420:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ILE:HD12	1:E:74:TYR:CD2	2.45	0.51
1:E:147:THR:HG21	1:E:152:TYR:HB3	1.93	0.51
1:A:41:TYR:CE1	1:A:110:LEU:HD12	2.45	0.50
1:A:147:THR:HG21	1:A:152:TYR:HB3	1.91	0.50
1:A:149:MET:HB3	1:A:150:PRO:HD2	1.93	0.50
1:D:72:TYR:CD2	1:D:72:TYR:O	2.63	0.50
1:E:180:ASP:OD2	1:E:180:ASP:C	2.49	0.50
1:E:233:HIS:HB2	1:E:312:ARG:NH1	2.26	0.50
2:R:18:C:O2'	2:R:19:C:H5'	2.11	0.50
1:C:155:LYS:NZ	2:R:17:C:OP2	2.39	0.50
1:C:184:VAL:HG11	1:D:166:MET:H	1.76	0.50
1:D:31:TYR:C	1:D:33:ARG:H	2.14	0.50
1:D:316:ALA:HA	1:D:317:ARG:CZ	2.41	0.50
1:E:70:ASN:HD22	1:E:70:ASN:H	1.58	0.50
1:B:323:GLU:OE1	1:C:239:GLY:HA3	2.11	0.50
1:E:172:GLU:HB3	1:E:173:PRO:CD	2.41	0.50
1:E:177:GLU:HG2	1:E:178:GLY:N	2.26	0.50
1:E:253:GLU:OE2	1:E:253:GLU:N	2.41	0.50
1:A:218:ILE:C	1:A:220:SER:H	2.15	0.50
1:B:323:GLU:O	1:B:327:LEU:HD22	2.11	0.50
2:R:10:C:H5"	2:R:11:C:OP2	2.11	0.50
2:R:34:C:O2	2:R:34:C:O4'	2.28	0.50
1:B:199:ASP:HB2	1:B:217:THR:HG23	1.93	0.50
1:E:354:LYS:CE	1:E:356:THR:HA	2.33	0.50
1:C:295:PRO:HB2	1:C:322:ILE:CG2	2.41	0.50
1:D:328:THR:HG21	1:D:415:TYR:OH	2.11	0.50
1:A:172:GLU:HB3	1:A:173:PRO:CD	2.42	0.50
1:B:72:TYR:CD2	1:B:72:TYR:C	2.82	0.50
1:B:151:GLU:O	1:B:155:LYS:HB2	2.12	0.50
1:C:60:LYS:O	1:C:61:SER:CB	2.52	0.50
1:C:181:ILE:H	1:C:181:ILE:CD1	2.17	0.50
1:A:230:THR:HG21	1:A:298:HIS:ND1	2.27	0.49
1:A:262:MET:HA	1:A:262:MET:CE	2.42	0.49
1:A:314:ARG:O	1:A:413:GLY:HA3	2.12	0.49
1:B:184:VAL:CG1	1:C:165:LYS:HA	2.41	0.49
1:B:240:MET:HE3	1:B:244:ASP:HB3	1.94	0.49
1:C:230:THR:HG21	1:C:298:HIS:ND1	2.26	0.49
1:E:136:LEU:C	1:E:136:LEU:HD23	2.32	0.49
1:A:81:ARG:HB2	1:A:208:HIS:HE2	1.75	0.49
1:B:105:PHE:C	1:B:107:LEU:N	2.66	0.49
1:C:72:TYR:CD2	1:C:72:TYR:C	2.83	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:PHE:CE2	1:E:267:GLU:HG3	2.47	0.49
1:A:177:GLU:HG2	1:A:178:GLY:N	2.27	0.49
1:B:14:ILE:HD11	1:C:259:VAL:HA	1.94	0.49
1:B:68:HIS:CE1	1:B:117:LEU:HG	2.46	0.49
1:B:199:ASP:CB	1:B:217:THR:HG23	2.41	0.49
1:D:170:GLN:O	1:D:171:PHE:HB3	2.13	0.49
1:D:179:ARG:HA	1:D:183:ASP:OD1	2.12	0.49
1:E:65:SER:HB3	1:E:68:HIS:ND1	2.27	0.49
1:E:153:ARG:NH1	1:E:176:PRO:O	2.45	0.49
1:E:203:HIS:HD2	1:E:272:ASP:OD1	1.94	0.49
1:B:37:GLU:HB2	1:B:108:VAL:HG21	1.95	0.49
1:C:293:LYS:C	1:C:295:PRO:HD3	2.32	0.49
1:D:38:ILE:HD11	1:D:107:LEU:O	2.11	0.49
1:E:38:ILE:HD11	1:E:107:LEU:O	2.12	0.49
1:E:149:MET:HB3	1:E:150:PRO:HD2	1.95	0.49
1:E:370:PRO:HD3	1:E:381:TRP:CG	2.47	0.49
1:A:149:MET:C	1:A:151:GLU:N	2.66	0.49
1:A:165:LYS:HG3	1:E:184:VAL:HG13	1.94	0.49
1:B:177:GLU:HG2	1:B:178:GLY:N	2.28	0.49
1:B:379:LEU:CD1	1:C:346:GLN:HB2	2.42	0.49
1:C:233:HIS:HB2	1:C:312:ARG:NH1	2.27	0.49
1:D:8:ILE:HG13	1:D:8:ILE:O	2.13	0.49
1:D:41:TYR:CE1	1:D:110:LEU:HD12	2.43	0.49
1:D:43:ASN:OD1	1:D:112:ALA:N	2.46	0.49
1:D:141:LEU:HD22	1:D:182:PHE:CE1	2.47	0.49
1:D:298:HIS:NE2	1:D:317:ARG:NH1	2.59	0.49
1:A:151:GLU:O	1:A:155:LYS:HB2	2.12	0.49
1:A:364:LEU:O	1:A:365:THR:C	2.50	0.49
1:D:122:SER:O	1:D:123:ASP:HB2	2.10	0.49
1:D:230:THR:HB	1:D:302:GLN:OE1	2.12	0.49
1:E:8:ILE:O	1:E:8:ILE:HG13	2.11	0.49
1:A:45:THR:H	1:A:111:LYS:HZ1	1.61	0.49
1:A:72:TYR:O	1:A:72:TYR:CD2	2.65	0.49
1:A:385:GLN:O	1:A:386:ASN:HB2	2.13	0.49
1:B:149:MET:O	1:B:152:TYR:CD2	2.65	0.49
1:C:412:ILE:HD12	1:C:412:ILE:C	2.32	0.49
1:D:172:GLU:HB3	1:D:173:PRO:CD	2.42	0.49
1:E:117:LEU:N	1:E:117:LEU:HD23	2.28	0.49
1:C:177:GLU:HG2	1:C:178:GLY:N	2.28	0.49
1:A:122:SER:O	1:A:123:ASP:HB2	2.12	0.49
1:A:149:MET:C	1:A:152:TYR:CE2	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PRO:HD3	1:A:152:TYR:OH	2.12	0.49
1:A:239:GLY:HA3	1:E:323:GLU:OE1	2.12	0.49
1:C:130:ASP:C	1:C:132:LYS:N	2.65	0.49
1:E:46:LYS:HD3	1:E:46:LYS:N	2.26	0.49
1:A:27:TYR:HB3	1:A:266:GLN:HE22	1.78	0.49
1:A:38:ILE:HD11	1:A:107:LEU:O	2.13	0.49
1:B:54:TYR:CD1	1:B:118:PRO:HB2	2.48	0.49
1:C:223:LYS:O	1:C:224:ASP:HB2	2.13	0.49
1:D:212:SER:HA	2:R:9:C:O2	2.12	0.49
1:E:72:TYR:O	1:E:72:TYR:CD2	2.66	0.49
1:A:15:VAL:O	1:A:17:LYS:HG2	2.12	0.48
1:B:122:SER:O	1:B:123:ASP:HB2	2.12	0.48
1:B:130:ASP:C	1:B:132:LYS:N	2.65	0.48
1:B:354:LYS:CE	1:B:356:THR:HA	2.37	0.48
1:B:376:VAL:HG13	1:C:354:LYS:CB	2.39	0.48
1:D:165:LYS:O	1:D:167:ILE:CD1	2.58	0.48
1:D:295:PRO:HB2	1:D:322:ILE:CG2	2.43	0.48
1:E:37:GLU:HB2	1:E:108:VAL:HG21	1.95	0.48
1:B:317:ARG:CD	1:B:317:ARG:H	2.25	0.48
1:C:141:LEU:HD22	1:C:182:PHE:CE1	2.47	0.48
1:D:199:ASP:CB	1:D:217:THR:HG23	2.43	0.48
1:E:43:ASN:OD1	1:E:112:ALA:N	2.46	0.48
2:R:18:C:H5'	2:R:18:C:C6	2.48	0.48
1:A:241:SER:OG	1:A:243:GLU:HG2	2.14	0.48
1:A:295:PRO:HB2	1:A:322:ILE:CG2	2.42	0.48
1:B:240:MET:HE3	1:B:244:ASP:CB	2.42	0.48
1:C:166:MET:HB2	1:C:167:ILE:CD1	2.43	0.48
1:C:180:ASP:OD2	1:C:180:ASP:O	2.31	0.48
1:C:401:VAL:HG21	1:C:420:PHE:HB2	1.94	0.48
1:B:179:ARG:HA	1:B:183:ASP:OD1	2.12	0.48
1:C:37:GLU:HB2	1:C:108:VAL:HG21	1.95	0.48
1:C:356:THR:CG2	1:C:357:PRO:HD3	2.29	0.48
1:D:151:GLU:O	1:D:155:LYS:HB2	2.13	0.48
1:A:18:LEU:HD12	1:B:232:GLY:HA2	1.95	0.48
1:B:36:LYS:HG3	1:B:93:ILE:HD11	1.95	0.48
1:B:148:GLN:O	1:B:152:TYR:CE2	2.65	0.48
1:B:149:MET:HB3	1:B:150:PRO:HD2	1.95	0.48
1:B:165:LYS:HB2	1:B:165:LYS:HZ2	1.78	0.48
1:C:68:HIS:CE1	1:C:117:LEU:HG	2.48	0.48
1:C:262:MET:HA	1:C:262:MET:CE	2.43	0.48
1:C:380:GLY:CA	1:D:354:LYS:HZ3	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:SER:O	1:E:123:ASP:HB2	2.12	0.48
2:R:44:C:H5”	2:R:45:C:OP2	2.12	0.48
1:B:253:GLU:HA	1:B:256:ASP:HB2	1.95	0.48
1:B:385:GLN:O	1:B:386:ASN:HB2	2.14	0.48
1:D:68:HIS:CE1	1:D:118:PRO:HD2	2.49	0.48
1:A:165:LYS:CB	1:A:165:LYS:HZ3	2.27	0.48
1:B:147:THR:HG21	1:B:152:TYR:HB3	1.94	0.48
1:D:149:MET:HB3	1:D:150:PRO:HD2	1.95	0.48
1:A:253:GLU:HA	1:A:256:ASP:HB2	1.95	0.48
1:B:180:ASP:C	1:B:180:ASP:OD2	2.50	0.48
1:C:238:THR:C	1:C:240:MET:H	2.16	0.48
1:A:293:LYS:C	1:A:295:PRO:HD3	2.35	0.48
1:A:412:ILE:HD12	1:A:412:ILE:C	2.34	0.48
1:C:59:LEU:HB3	1:C:172:GLU:HG2	1.96	0.48
1:E:147:THR:CG2	1:E:152:TYR:HB3	2.44	0.48
1:E:255:ALA:O	1:E:259:VAL:HG23	2.14	0.48
1:B:199:ASP:OD1	1:B:217:THR:HG23	2.13	0.48
1:B:317:ARG:NE	2:R:22:C:O2’	2.47	0.48
1:C:136:LEU:HD23	1:C:136:LEU:O	2.14	0.48
1:C:283:LEU:HD23	1:C:283:LEU:N	2.29	0.48
1:D:68:HIS:CE1	1:D:117:LEU:HG	2.49	0.48
1:A:230:THR:HB	1:A:302:GLN:OE1	2.14	0.47
1:C:172:GLU:HB3	1:C:173:PRO:HD3	1.96	0.47
1:C:179:ARG:HA	1:C:183:ASP:OD1	2.13	0.47
1:D:59:LEU:HB3	1:D:172:GLU:HG2	1.96	0.47
1:D:78:LYS:O	1:D:80:ILE:HD12	2.14	0.47
1:D:253:GLU:HA	1:D:256:ASP:HB2	1.95	0.47
1:E:409:GLU:HG3	1:E:414:LYS:HD3	1.96	0.47
2:R:27:C:H2’	2:R:28:C:O4’	2.13	0.47
1:A:46:LYS:HD3	1:A:46:LYS:N	2.27	0.47
1:A:147:THR:CG2	1:A:152:TYR:HB3	2.44	0.47
1:B:43:ASN:OD1	1:B:112:ALA:HB3	2.15	0.47
1:B:295:PRO:HB2	1:B:322:ILE:HG21	1.96	0.47
1:B:412:ILE:C	1:B:412:ILE:HD12	2.34	0.47
1:C:141:LEU:HD22	1:C:182:PHE:CD1	2.49	0.47
1:D:36:LYS:HG3	1:D:93:ILE:HD11	1.96	0.47
1:E:141:LEU:HD22	1:E:182:PHE:CE1	2.49	0.47
1:A:59:LEU:HB3	1:A:172:GLU:HG2	1.97	0.47
1:A:70:ASN:HD22	1:A:70:ASN:H	1.60	0.47
1:A:136:LEU:HD23	1:A:136:LEU:O	2.15	0.47
1:C:317:ARG:CZ	2:R:13:C:O2’	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:LYS:HG2	1:C:402:MET:CE	2.43	0.47
1:D:153:ARG:CZ	1:D:176:PRO:HA	2.44	0.47
1:E:144:VAL:O	1:E:147:THR:HG22	2.14	0.47
1:A:45:THR:H	1:A:111:LYS:NZ	2.12	0.47
1:A:180:ASP:OD2	1:A:180:ASP:O	2.32	0.47
1:A:409:GLU:HG3	1:A:414:LYS:HD3	1.96	0.47
1:D:385:GLN:O	1:D:386:ASN:HB2	2.14	0.47
1:E:398:LYS:HG2	1:E:402:MET:CE	2.43	0.47
1:A:36:LYS:HG3	1:A:93:ILE:HD11	1.97	0.47
1:A:59:LEU:O	1:A:61:SER:N	2.47	0.47
1:A:141:LEU:HD22	1:A:182:PHE:CE1	2.50	0.47
1:D:354:LYS:CE	1:D:356:THR:HA	2.34	0.47
1:E:54:TYR:OH	1:E:120:GLY:N	2.48	0.47
1:E:163:GLN:C	1:E:165:LYS:N	2.67	0.47
1:E:212:SER:HA	2:R:45:C:C6	2.50	0.47
1:A:8:ILE:HG13	1:A:8:ILE:O	2.15	0.47
1:B:150:PRO:N	1:B:152:TYR:CZ	2.83	0.47
1:B:171:PHE:CD2	1:B:172:GLU:N	2.82	0.47
1:C:105:PHE:C	1:C:107:LEU:N	2.67	0.47
1:C:409:GLU:HG3	1:C:414:LYS:HD3	1.95	0.47
1:D:223:LYS:O	1:D:224:ASP:HB2	2.15	0.47
1:A:68:HIS:CE1	1:A:117:LEU:HG	2.48	0.47
1:A:149:MET:C	1:A:152:TYR:CZ	2.88	0.47
1:A:149:MET:O	1:A:152:TYR:CG	2.68	0.47
1:A:328:THR:HG21	1:A:415:TYR:OH	2.15	0.47
1:B:382:PHE:HE1	1:B:393:MET:HE1	1.78	0.47
1:C:43:ASN:OD1	1:C:112:ALA:HB3	2.15	0.47
1:C:78:LYS:O	1:C:80:ILE:HD12	2.14	0.47
1:C:78:LYS:O	1:C:80:ILE:N	2.47	0.47
1:C:122:SER:O	1:C:123:ASP:HB2	2.14	0.47
1:C:376:VAL:HG13	1:D:354:LYS:CA	2.43	0.47
1:D:136:LEU:HD23	1:D:136:LEU:O	2.15	0.47
1:D:177:GLU:HG2	1:D:178:GLY:N	2.30	0.47
1:E:177:GLU:HG2	1:E:178:GLY:H	1.80	0.47
1:E:181:ILE:HB	1:E:182:PHE:CD2	2.50	0.47
1:A:29:ALA:C	1:A:31:TYR:H	2.13	0.47
1:A:79:ASP:HB2	1:A:81:ARG:NE	2.30	0.47
1:A:89:SER:O	1:A:90:SER:CB	2.63	0.47
1:C:149:MET:C	1:C:151:GLU:N	2.63	0.47
1:E:55:VAL:HG12	1:E:64:VAL:HG21	1.96	0.47
1:E:215:TYR:C	1:E:215:TYR:CD2	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:VAL:HG12	1:D:64:VAL:HG21	1.97	0.47
1:E:163:GLN:O	1:E:165:LYS:N	2.48	0.47
2:R:21:C:H5"	2:R:21:C:C6	2.39	0.47
1:A:223:LYS:O	1:A:224:ASP:HB2	2.14	0.47
1:B:38:ILE:HD11	1:B:107:LEU:O	2.14	0.47
1:C:148:GLN:O	1:C:152:TYR:CE2	2.68	0.47
1:C:253:GLU:HA	1:C:256:ASP:HB2	1.97	0.47
1:D:147:THR:HG21	1:D:152:TYR:HA	1.96	0.47
1:D:364:LEU:HB3	1:D:368:ALA:CB	2.45	0.47
1:E:41:TYR:CE1	1:E:110:LEU:HD12	2.44	0.47
1:E:68:HIS:CE1	1:E:117:LEU:HG	2.49	0.47
1:B:81:ARG:HB2	1:B:208:HIS:NE2	2.29	0.46
1:B:86:LYS:HB3	1:B:87:ASP:H	1.56	0.46
1:B:208:HIS:CE1	1:B:210:CYS:HB2	2.50	0.46
1:C:196:ALA:HB3	1:C:281:PHE:CE1	2.51	0.46
1:D:293:LYS:C	1:D:295:PRO:HD3	2.35	0.46
1:E:28:PRO:O	1:E:31:TYR:HB3	2.15	0.46
1:E:293:LYS:C	1:E:295:PRO:HD3	2.36	0.46
1:E:385:GLN:O	1:E:386:ASN:HB2	2.15	0.46
1:A:18:LEU:HD12	1:B:232:GLY:CA	2.45	0.46
1:B:283:LEU:N	1:B:283:LEU:HD23	2.29	0.46
1:E:136:LEU:HD23	1:E:136:LEU:O	2.16	0.46
1:E:179:ARG:HA	1:E:183:ASP:OD1	2.15	0.46
1:B:59:LEU:HB3	1:B:172:GLU:HG2	1.97	0.46
1:B:70:ASN:HD22	1:B:70:ASN:H	1.60	0.46
1:B:172:GLU:HB3	1:B:173:PRO:CD	2.45	0.46
1:B:293:LYS:C	1:B:295:PRO:HD3	2.36	0.46
1:B:356:THR:CG2	1:B:357:PRO:HD3	2.31	0.46
1:C:153:ARG:NH1	1:C:176:PRO:O	2.44	0.46
1:E:72:TYR:CD2	1:E:72:TYR:C	2.86	0.46
1:E:107:LEU:HD23	1:E:274:TYR:HE2	1.81	0.46
1:A:81:ARG:CD	1:A:208:HIS:HE2	2.28	0.46
1:A:167:ILE:O	1:A:168:ASN:HB2	2.16	0.46
1:A:179:ARG:HA	1:A:183:ASP:OD1	2.15	0.46
1:C:14:ILE:CD1	1:D:259:VAL:HA	2.44	0.46
1:D:151:GLU:HG2	1:D:155:LYS:HD3	1.98	0.46
1:E:283:LEU:HD23	1:E:283:LEU:N	2.30	0.46
1:E:317:ARG:HG3	2:R:40:C:C2	2.49	0.46
1:A:200:MET:HB2	1:A:277:TYR:CE2	2.51	0.46
1:A:237:ILE:CD1	1:A:310:SER:HB2	2.45	0.46
1:B:54:TYR:OH	1:B:120:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLY:O	1:B:63:ASN:O	2.34	0.46
1:B:81:ARG:CD	1:B:208:HIS:HE2	2.29	0.46
1:C:147:THR:CG2	1:C:152:TYR:HB3	2.45	0.46
1:D:78:LYS:O	1:D:80:ILE:N	2.48	0.46
1:E:74:TYR:O	1:E:78:LYS:HD3	2.16	0.46
1:E:151:GLU:HA	1:E:154:LYS:HB3	1.98	0.46
1:A:177:GLU:HG2	1:A:178:GLY:H	1.80	0.46
1:B:230:THR:HB	1:B:302:GLN:OE1	2.15	0.46
1:C:181:ILE:HB	1:C:182:PHE:CD2	2.51	0.46
1:D:240:MET:HE3	1:D:240:MET:HB3	1.81	0.46
1:A:37:GLU:HB2	1:A:108:VAL:HG21	1.98	0.46
1:A:72:TYR:CD2	1:A:72:TYR:C	2.85	0.46
1:A:78:LYS:HE2	1:A:78:LYS:HB2	1.76	0.46
1:A:105:PHE:C	1:A:107:LEU:N	2.64	0.46
1:C:14:ILE:HD12	1:D:259:VAL:HG22	1.98	0.46
1:C:45:THR:O	1:C:46:LYS:HD3	2.15	0.46
1:C:240:MET:HE3	1:C:244:ASP:CB	2.46	0.46
1:D:45:THR:O	1:D:46:LYS:HD3	2.15	0.46
1:D:365:THR:HG23	1:D:366:THR:H	1.81	0.46
1:E:37:GLU:CB	1:E:108:VAL:HG11	2.40	0.46
1:E:226:ALA:HB2	2:R:40:C:H5'	1.98	0.46
1:A:153:ARG:CZ	1:A:176:PRO:HA	2.46	0.46
1:A:167:ILE:HG22	1:A:169:GLU:CD	2.36	0.46
1:A:253:GLU:OE2	1:A:253:GLU:N	2.44	0.46
1:B:68:HIS:CE1	1:B:118:PRO:HD2	2.51	0.46
1:B:147:THR:CG2	1:B:152:TYR:HB3	2.46	0.46
1:C:41:TYR:CE1	1:C:110:LEU:HD12	2.47	0.46
1:C:107:LEU:HD23	1:C:274:TYR:HE2	1.80	0.46
1:B:149:MET:C	1:B:152:TYR:CZ	2.89	0.46
1:C:226:ALA:HB3	1:C:291:SER:HB3	1.98	0.46
1:D:81:ARG:HB2	1:D:208:HIS:NE2	2.31	0.46
1:A:55:VAL:HG12	1:A:64:VAL:HG21	1.97	0.46
1:A:65:SER:HB3	1:A:68:HIS:ND1	2.31	0.46
1:A:107:LEU:HD23	1:A:274:TYR:HE2	1.81	0.46
1:A:401:VAL:HG21	1:A:420:PHE:HB2	1.96	0.46
1:B:255:ALA:O	1:B:256:ASP:C	2.53	0.46
1:B:408:ARG:HD3	2:R:24:C:C4	2.51	0.46
1:D:144:VAL:O	1:D:147:THR:HG22	2.15	0.46
1:E:148:GLN:O	1:E:152:TYR:CE2	2.68	0.46
1:E:382:PHE:CD2	1:E:387:ARG:HA	2.50	0.46
2:R:9:C:C6	2:R:10:C:C5	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TYR:CE1	1:B:122:SER:HB2	2.51	0.45
1:B:203:HIS:HD2	1:B:272:ASP:OD1	1.98	0.45
1:B:401:VAL:HG21	1:B:420:PHE:HB2	1.96	0.45
1:D:37:GLU:HB2	1:D:108:VAL:HG21	1.98	0.45
1:D:181:ILE:HB	1:D:182:PHE:CD2	2.51	0.45
1:D:283:LEU:N	1:D:283:LEU:HD23	2.30	0.45
1:E:147:THR:HG21	1:E:152:TYR:HA	1.97	0.45
1:E:223:LYS:O	1:E:224:ASP:HB2	2.16	0.45
1:A:54:TYR:CD1	1:A:118:PRO:HB2	2.50	0.45
1:B:107:LEU:HD23	1:B:274:TYR:HE2	1.80	0.45
1:C:119:ASP:OD1	1:C:119:ASP:N	2.50	0.45
1:C:177:GLU:HG2	1:C:178:GLY:H	1.81	0.45
1:E:172:GLU:HB3	1:E:173:PRO:HD3	1.98	0.45
1:B:151:GLU:HA	1:B:154:LYS:HB3	1.99	0.45
1:C:317:ARG:H	1:C:317:ARG:CD	2.30	0.45
1:D:42:ILE:HD12	1:D:74:TYR:CB	2.38	0.45
1:D:226:ALA:HB2	2:R:4:C:O5'	2.17	0.45
1:D:317:ARG:CZ	1:D:317:ARG:N	2.74	0.45
1:E:167:ILE:HG22	1:E:168:ASN:H	1.80	0.45
1:E:409:GLU:HA	1:E:414:LYS:HD2	1.99	0.45
1:B:153:ARG:NH1	1:B:176:PRO:O	2.47	0.45
1:B:317:ARG:NH2	2:R:23:C:C5'	2.59	0.45
1:C:70:ASN:HD22	1:C:70:ASN:H	1.65	0.45
1:C:81:ARG:CD	1:C:208:HIS:HE2	2.29	0.45
1:D:89:SER:O	1:D:90:SER:CB	2.64	0.45
1:D:240:MET:HE3	1:D:244:ASP:CB	2.47	0.45
1:D:409:GLU:HG3	1:D:414:LYS:HD3	1.97	0.45
1:E:328:THR:HG21	1:E:415:TYR:OH	2.16	0.45
1:A:283:LEU:N	1:A:283:LEU:HD23	2.32	0.45
1:B:385:GLN:HG2	1:B:390:THR:CG2	2.47	0.45
1:C:15:VAL:O	1:C:17:LYS:HG2	2.17	0.45
1:D:74:TYR:O	1:D:78:LYS:HD3	2.16	0.45
1:D:238:THR:C	1:D:240:MET:H	2.20	0.45
2:R:32:C:N4	2:R:34:C:C5	2.84	0.45
1:A:59:LEU:O	1:A:61:SER:O	2.34	0.45
1:C:3:VAL:O	1:C:4:THR:HB	2.15	0.45
1:D:141:LEU:HD22	1:D:182:PHE:CD1	2.52	0.45
1:D:172:GLU:HB3	1:D:173:PRO:HD3	1.98	0.45
1:E:27:TYR:HB3	1:E:266:GLN:HE22	1.82	0.45
1:E:55:VAL:O	1:E:56:TYR:C	2.55	0.45
1:B:41:TYR:CE1	1:B:110:LEU:HD12	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:PRO:HD3	1:C:152:TYR:OH	2.17	0.45
1:E:253:GLU:HA	1:E:256:ASP:HB2	1.98	0.45
1:A:313:ALA:O	1:A:412:ILE:HD11	2.17	0.45
1:B:8:ILE:HG13	1:B:8:ILE:O	2.17	0.45
1:B:79:ASP:HB2	1:B:81:ARG:NE	2.32	0.45
1:C:38:ILE:O	1:C:108:VAL:HB	2.16	0.45
1:D:54:TYR:CD1	1:D:118:PRO:HB2	2.52	0.45
1:D:196:ALA:HB3	1:D:281:PHE:CE1	2.52	0.45
1:E:81:ARG:CD	1:E:208:HIS:HE2	2.29	0.45
1:A:22:GLU:HB3	1:B:206:LYS:NZ	2.32	0.45
1:A:163:GLN:N	1:A:163:GLN:CD	2.71	0.45
1:A:238:THR:C	1:A:240:MET:H	2.20	0.45
1:A:382:PHE:CD2	1:A:387:ARG:HA	2.52	0.45
1:B:91:PHE:CE2	1:B:267:GLU:HG3	2.52	0.45
1:C:184:VAL:HG11	1:D:166:MET:N	2.32	0.45
1:C:275:MET:HB3	1:C:276:PRO:HD3	1.99	0.45
1:E:105:PHE:C	1:E:107:LEU:N	2.67	0.45
1:E:153:ARG:CZ	1:E:176:PRO:HA	2.47	0.45
1:A:167:ILE:CG2	1:A:169:GLU:HG2	2.43	0.45
1:A:181:ILE:HB	1:A:182:PHE:CD2	2.52	0.45
1:A:241:SER:O	1:A:245:VAL:HG23	2.17	0.45
1:A:275:MET:HB3	1:A:276:PRO:HD3	1.98	0.45
1:E:150:PRO:HD3	1:E:152:TYR:OH	2.17	0.45
1:E:218:ILE:C	1:E:220:SER:H	2.20	0.45
1:E:259:VAL:O	1:E:260:GLN:C	2.54	0.45
1:A:144:VAL:O	1:A:147:THR:HG22	2.17	0.44
1:B:165:LYS:O	1:B:167:ILE:CD1	2.65	0.44
1:D:215:TYR:CD2	1:D:215:TYR:C	2.90	0.44
1:E:401:VAL:HG21	1:E:420:PHE:HB2	1.98	0.44
1:A:28:PRO:O	1:A:29:ALA:C	2.55	0.44
1:C:144:VAL:O	1:C:147:THR:HG22	2.17	0.44
1:D:397:ALA:O	1:D:401:VAL:HG22	2.17	0.44
1:E:31:TYR:C	1:E:33:ARG:H	2.20	0.44
1:E:168:ASN:O	1:E:169:GLU:HB2	2.17	0.44
1:E:366:THR:C	1:E:368:ALA:H	2.21	0.44
1:A:184:VAL:HG13	1:B:165:LYS:HG3	1.99	0.44
1:B:218:ILE:C	1:B:220:SER:H	2.21	0.44
1:E:29:ALA:HB2	1:E:91:PHE:HE2	1.81	0.44
1:A:45:THR:O	1:A:46:LYS:HD3	2.18	0.44
1:B:147:THR:HG21	1:B:152:TYR:HA	1.98	0.44
1:B:275:MET:HB3	1:B:276:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ARG:HB2	1:C:208:HIS:NE2	2.32	0.44
1:C:208:HIS:CE1	1:C:210:CYS:HB2	2.52	0.44
1:E:149:MET:HG3	2:R:42:C:C6	2.53	0.44
1:E:317:ARG:HH21	2:R:41:C:H5'	1.73	0.44
1:E:364:LEU:O	1:E:365:THR:C	2.56	0.44
1:A:208:HIS:CE1	1:A:210:CYS:HB2	2.52	0.44
1:A:364:LEU:HD22	1:A:368:ALA:HB2	2.00	0.44
1:B:409:GLU:HG3	1:B:414:LYS:HD3	1.99	0.44
1:C:218:ILE:C	1:C:220:SER:H	2.20	0.44
1:C:397:ALA:O	1:C:401:VAL:HG22	2.17	0.44
1:E:46:LYS:HD3	1:E:46:LYS:HA	1.70	0.44
1:A:147:THR:HG21	1:A:152:TYR:HA	1.99	0.44
1:A:172:GLU:HB3	1:A:173:PRO:HD3	1.99	0.44
1:A:376:VAL:HG13	1:B:354:LYS:CB	2.45	0.44
1:B:103:GLY:N	1:B:106:ASP:OD2	2.48	0.44
1:B:328:THR:HG21	1:B:415:TYR:OH	2.17	0.44
1:C:54:TYR:OH	1:C:120:GLY:N	2.50	0.44
1:C:354:LYS:CE	1:C:356:THR:HA	2.38	0.44
1:D:14:ILE:HG23	1:D:16:PRO:HD3	1.99	0.44
1:D:91:PHE:CE2	1:D:267:GLU:HG3	2.51	0.44
1:E:45:THR:O	1:E:46:LYS:HD3	2.18	0.44
1:A:18:LEU:CD1	1:B:232:GLY:HA2	2.48	0.44
1:B:177:GLU:HG2	1:B:178:GLY:H	1.81	0.44
1:B:238:THR:C	1:B:240:MET:H	2.21	0.44
1:C:55:VAL:HG12	1:C:64:VAL:HG21	1.99	0.44
1:C:249:ILE:HD13	1:C:254:VAL:HG12	1.99	0.44
1:E:365:THR:HG23	1:E:366:THR:H	1.83	0.44
1:A:150:PRO:N	1:A:152:TYR:CZ	2.86	0.44
1:B:153:ARG:HH12	1:B:177:GLU:HB2	1.83	0.44
1:C:90:SER:O	1:C:91:PHE:HB2	2.18	0.44
1:C:253:GLU:OE2	1:C:253:GLU:N	2.44	0.44
1:D:113:LEU:N	1:D:113:LEU:HD23	2.33	0.44
1:D:181:ILE:H	1:D:181:ILE:CD1	2.26	0.44
1:E:196:ALA:HB3	1:E:281:PHE:CE1	2.53	0.44
1:E:275:MET:SD	1:E:275:MET:C	2.96	0.44
1:A:151:GLU:HA	1:A:154:LYS:HB3	2.00	0.44
1:B:144:VAL:O	1:B:147:THR:HG22	2.17	0.44
1:B:181:ILE:HB	1:B:182:PHE:CD2	2.53	0.44
1:C:7:ARG:NH2	1:D:256:ASP:OD2	2.51	0.44
1:C:151:GLU:HA	1:C:154:LYS:HB3	2.00	0.44
1:C:165:LYS:CB	1:C:165:LYS:HZ3	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:LEU:HD23	1:D:274:TYR:HE2	1.83	0.44
1:E:79:ASP:HB2	1:E:81:ARG:NE	2.32	0.44
1:E:81:ARG:HB2	1:E:208:HIS:NE2	2.33	0.44
2:R:9:C:H2'	2:R:10:C:O4'	2.17	0.44
1:A:78:LYS:O	1:A:80:ILE:HD12	2.18	0.43
1:B:141:LEU:HD22	1:B:182:PHE:CE1	2.53	0.43
1:B:342:ALA:HB1	1:B:344:LEU:HD23	1.99	0.43
1:D:54:TYR:CE1	1:D:122:SER:HB2	2.53	0.43
1:D:54:TYR:OH	1:D:120:GLY:N	2.50	0.43
1:E:68:HIS:CE1	1:E:118:PRO:HD2	2.53	0.43
1:E:149:MET:C	1:E:152:TYR:CE2	2.91	0.43
1:E:238:THR:C	1:E:240:MET:H	2.21	0.43
1:A:409:GLU:HA	1:A:414:LYS:HD2	2.00	0.43
1:B:349:CYS:SG	1:E:8:ILE:CG2	3.02	0.43
1:D:46:LYS:HD3	1:D:46:LYS:N	2.24	0.43
1:E:141:LEU:HD22	1:E:182:PHE:CD1	2.53	0.43
1:E:151:GLU:HG2	1:E:155:LYS:HD3	1.99	0.43
1:B:29:ALA:C	1:B:31:TYR:N	2.72	0.43
1:B:65:SER:HB3	1:B:68:HIS:ND1	2.33	0.43
1:C:18:LEU:CD1	1:D:232:GLY:HA2	2.49	0.43
1:C:215:TYR:CD2	1:C:215:TYR:C	2.91	0.43
1:C:228:LEU:HD22	1:C:228:LEU:O	2.18	0.43
1:D:43:ASN:OD1	1:D:112:ALA:HB3	2.18	0.43
1:D:323:GLU:O	1:D:327:LEU:HD22	2.18	0.43
1:E:149:MET:O	1:E:152:TYR:CD2	2.71	0.43
1:E:410:LYS:HZ1	2:R:40:C:H42	1.65	0.43
2:R:39:C:H5'	2:R:40:C:OP2	2.19	0.43
1:B:170:GLN:HE21	1:B:170:GLN:HB3	1.59	0.43
1:B:303:LEU:CD2	1:B:328:THR:HA	2.48	0.43
1:D:153:ARG:NH2	1:D:176:PRO:HA	2.33	0.43
1:E:199:ASP:OD1	1:E:217:THR:HG23	2.18	0.43
1:E:342:ALA:HB1	1:E:344:LEU:HD23	2.00	0.43
2:R:40:C:O2	2:R:40:C:C2'	2.66	0.43
1:A:168:ASN:C	1:A:169:GLU:OE2	2.57	0.43
1:B:45:THR:O	1:B:46:LYS:HD3	2.18	0.43
1:B:376:VAL:HG13	1:C:354:LYS:CA	2.48	0.43
1:B:383:GLU:CG	1:C:354:LYS:HE2	2.46	0.43
1:D:123:ASP:C	1:D:125:SER:H	2.22	0.43
1:D:398:LYS:HG2	1:D:402:MET:CE	2.47	0.43
1:A:343:ASP:HB2	1:A:344:LEU:H	1.68	0.43
1:B:78:LYS:O	1:B:80:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:N	1:B:135:PRO:CD	2.82	0.43
1:B:316:ALA:HA	1:B:317:ARG:CZ	2.47	0.43
1:C:149:MET:C	1:C:152:TYR:CE2	2.91	0.43
1:C:247:THR:HA	1:D:348:PHE:HB2	2.01	0.43
1:D:4:THR:HG23	1:D:4:THR:O	2.18	0.43
1:D:149:MET:O	1:D:152:TYR:CD2	2.72	0.43
1:D:151:GLU:HA	1:D:154:LYS:HB3	2.01	0.43
2:R:9:C:C5	2:R:10:C:C5	3.06	0.43
1:A:167:ILE:O	1:A:169:GLU:OE1	2.37	0.43
1:A:364:LEU:O	1:A:366:THR:N	2.52	0.43
1:B:149:MET:O	1:B:152:TYR:CG	2.71	0.43
1:B:171:PHE:CZ	1:B:173:PRO:CG	3.00	0.43
1:C:136:LEU:CD2	1:C:163:GLN:HE21	2.25	0.43
1:C:230:THR:HB	1:C:302:GLN:OE1	2.19	0.43
1:D:81:ARG:CD	1:D:208:HIS:HE2	2.32	0.43
1:D:105:PHE:C	1:D:107:LEU:N	2.70	0.43
1:D:164:CYS:HA	1:D:168:ASN:HA	2.00	0.43
1:B:19:PRO:CG	1:C:228:LEU:CD1	2.96	0.43
1:D:149:MET:C	1:D:152:TYR:CE2	2.92	0.43
1:D:233:HIS:HB2	1:D:312:ARG:NH1	2.33	0.43
1:E:230:THR:HB	1:E:302:GLN:OE1	2.18	0.43
1:A:54:TYR:OH	1:A:120:GLY:N	2.52	0.43
1:B:136:LEU:HD23	1:B:136:LEU:O	2.19	0.43
1:B:163:GLN:N	1:B:163:GLN:CD	2.73	0.43
1:B:228:LEU:O	1:B:228:LEU:HD22	2.19	0.43
1:B:366:THR:C	1:B:368:ALA:H	2.21	0.43
1:C:54:TYR:CE1	1:C:122:SER:HB2	2.53	0.43
1:C:79:ASP:HB2	1:C:81:ARG:NE	2.34	0.43
1:D:342:ALA:HB1	1:D:344:LEU:HD23	2.00	0.43
1:A:112:ALA:HB1	1:A:113:LEU:HD23	1.99	0.43
1:B:172:GLU:HB3	1:B:173:PRO:HD3	2.00	0.43
1:D:150:PRO:HD3	1:D:152:TYR:OH	2.19	0.43
2:R:10:C:C5'	2:R:11:C:OP2	2.67	0.43
1:A:385:GLN:HG2	1:A:390:THR:CG2	2.48	0.42
1:D:81:ARG:HD2	1:D:208:HIS:NE2	2.34	0.42
1:D:409:GLU:HA	1:D:414:LYS:HD2	2.01	0.42
1:D:421:ASP:O	1:D:422:LYS:HB3	2.19	0.42
1:E:87:ASP:O	1:E:88:TRP:HB2	2.18	0.42
1:E:165:LYS:HB2	1:E:165:LYS:HZ3	1.83	0.42
1:A:91:PHE:CE2	1:A:267:GLU:HG3	2.54	0.42
1:A:240:MET:HE3	1:A:244:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:MET:HE2	1:A:402:MET:HB3	1.90	0.42
1:D:218:ILE:C	1:D:220:SER:H	2.23	0.42
1:D:255:ALA:O	1:D:259:VAL:HG23	2.20	0.42
1:E:90:SER:O	1:E:91:PHE:HB2	2.18	0.42
1:A:55:VAL:HG12	1:A:64:VAL:CG2	2.49	0.42
1:B:4:THR:HG23	1:B:4:THR:O	2.20	0.42
1:B:55:VAL:HG12	1:B:64:VAL:HG21	2.00	0.42
1:B:214:ARG:O	1:B:215:TYR:C	2.55	0.42
1:C:38:ILE:CD1	1:C:107:LEU:O	2.67	0.42
1:C:241:SER:OG	1:C:243:GLU:HG2	2.19	0.42
1:D:202:PHE:CG	1:D:211:ALA:HA	2.54	0.42
1:D:356:THR:CG2	1:D:357:PRO:HD3	2.35	0.42
1:D:412:ILE:HD12	1:D:413:GLY:N	2.34	0.42
1:E:89:SER:O	1:E:90:SER:CB	2.64	0.42
1:A:54:TYR:CE1	1:A:122:SER:HB2	2.54	0.42
1:A:68:HIS:CE1	1:A:118:PRO:HD2	2.55	0.42
1:B:57:GLN:HE21	1:B:60:LYS:NZ	2.18	0.42
1:C:147:THR:HG21	1:C:152:TYR:HA	2.00	0.42
1:D:79:ASP:HB2	1:D:81:ARG:NE	2.34	0.42
1:E:356:THR:CG2	1:E:357:PRO:HD3	2.34	0.42
1:A:78:LYS:O	1:A:80:ILE:N	2.53	0.42
1:A:103:GLY:N	1:A:106:ASP:OD2	2.49	0.42
1:C:8:ILE:O	1:C:8:ILE:HG13	2.19	0.42
1:C:105:PHE:O	1:C:107:LEU:N	2.52	0.42
1:C:112:ALA:HB1	1:C:113:LEU:HD23	2.01	0.42
1:C:255:ALA:O	1:C:256:ASP:C	2.56	0.42
1:E:163:GLN:CD	1:E:163:GLN:N	2.73	0.42
1:B:196:ALA:HB3	1:B:281:PHE:CE1	2.55	0.42
1:C:170:GLN:HB3	1:C:171:PHE:H	1.42	0.42
1:D:55:VAL:HG12	1:D:64:VAL:CG2	2.50	0.42
1:D:224:ASP:HA	2:R:4:C:OP1	2.19	0.42
1:D:226:ALA:HB3	1:D:291:SER:HB3	2.02	0.42
1:E:54:TYR:CE1	1:E:122:SER:HB2	2.54	0.42
1:A:31:TYR:CD1	1:A:32:PHE:N	2.88	0.42
1:A:295:PRO:HB2	1:A:322:ILE:HG21	2.02	0.42
1:A:380:GLY:CA	1:B:354:LYS:HZ3	2.27	0.42
1:C:409:GLU:HA	1:C:414:LYS:HD2	2.02	0.42
1:D:90:SER:O	1:D:91:PHE:HB2	2.20	0.42
1:D:208:HIS:CE1	1:D:210:CYS:HB2	2.54	0.42
1:D:228:LEU:O	1:D:228:LEU:HD22	2.19	0.42
1:D:366:THR:C	1:D:368:ALA:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TYR:O	1:A:78:LYS:HD3	2.19	0.42
1:A:81:ARG:HB2	1:A:208:HIS:NE2	2.34	0.42
1:B:66:ILE:HD13	1:B:185:TRP:CD1	2.54	0.42
1:B:369:PRO:HB3	1:B:381:TRP:CZ2	2.55	0.42
1:C:255:ALA:O	1:C:259:VAL:HG23	2.20	0.42
1:D:263:LEU:HD12	1:D:263:LEU:HA	1.91	0.42
1:D:399:ARG:HB3	1:D:399:ARG:NH1	2.35	0.42
1:E:54:TYR:CD1	1:E:118:PRO:HB2	2.52	0.42
1:E:119:ASP:OD1	1:E:119:ASP:N	2.53	0.42
1:B:55:VAL:O	1:B:56:TYR:C	2.57	0.42
1:B:231:PHE:HB2	1:B:297:PHE:CZ	2.54	0.42
1:B:382:PHE:CD2	1:B:387:ARG:HA	2.55	0.42
1:C:103:GLY:N	1:C:106:ASP:OD2	2.47	0.42
1:D:65:SER:HB3	1:D:68:HIS:ND1	2.34	0.42
1:D:180:ASP:OD2	1:D:180:ASP:O	2.38	0.42
1:E:399:ARG:NH1	1:E:399:ARG:HB3	2.35	0.42
1:B:18:LEU:HD11	1:C:232:GLY:HA2	2.01	0.42
1:B:153:ARG:CZ	1:B:176:PRO:HA	2.50	0.42
1:B:237:ILE:CD1	1:B:310:SER:HB2	2.50	0.42
1:C:163:GLN:CD	1:C:163:GLN:N	2.73	0.42
1:D:253:GLU:CD	1:D:253:GLU:N	2.71	0.42
1:E:167:ILE:O	1:E:168:ASN:HB2	2.18	0.42
1:A:317:ARG:CD	2:R:31:C:H2'	2.48	0.41
1:C:65:SER:HB3	1:C:68:HIS:ND1	2.34	0.41
1:D:313:ALA:O	1:D:412:ILE:HD11	2.20	0.41
1:E:249:ILE:HD13	1:E:254:VAL:HG12	2.02	0.41
1:E:397:ALA:O	1:E:401:VAL:HG22	2.20	0.41
1:A:37:GLU:CB	1:A:108:VAL:HG11	2.44	0.41
1:B:74:TYR:O	1:B:78:LYS:HD3	2.20	0.41
1:C:42:ILE:O	1:C:43:ASN:O	2.38	0.41
1:C:238:THR:O	1:C:240:MET:N	2.53	0.41
1:C:298:HIS:NE2	1:C:317:ARG:NH1	2.66	0.41
1:D:195:VAL:CG2	1:D:196:ALA:N	2.82	0.41
1:D:255:ALA:O	1:D:256:ASP:C	2.56	0.41
1:D:397:ALA:HB1	1:D:420:PHE:CG	2.55	0.41
1:E:190:ASN:O	1:E:194:ILE:HG13	2.20	0.41
1:E:363:GLY:C	1:E:365:THR:H	2.23	0.41
1:E:385:GLN:HG2	1:E:390:THR:CG2	2.51	0.41
1:A:43:ASN:OD1	1:A:112:ALA:HB3	2.20	0.41
1:A:73:LEU:O	1:A:74:TYR:C	2.59	0.41
1:C:18:LEU:HD12	1:D:232:GLY:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:ILE:N	1:E:93:ILE:HD12	2.35	0.41
1:E:160:LEU:HA	1:E:163:GLN:OE1	2.20	0.41
1:E:255:ALA:O	1:E:256:ASP:C	2.59	0.41
1:E:369:PRO:HA	1:E:370:PRO:HD3	1.81	0.41
2:R:25:C:H2'	2:R:26:C:H6	1.82	0.41
1:A:356:THR:CG2	1:A:357:PRO:HD3	2.36	0.41
1:B:38:ILE:O	1:B:108:VAL:HB	2.21	0.41
1:B:90:SER:O	1:B:91:PHE:HB2	2.20	0.41
1:B:105:PHE:O	1:B:107:LEU:N	2.51	0.41
1:B:158:ASP:C	1:B:160:LEU:H	2.24	0.41
1:C:55:VAL:O	1:C:56:TYR:C	2.58	0.41
1:C:149:MET:O	1:C:152:TYR:CD2	2.74	0.41
1:C:249:ILE:HD12	1:D:348:PHE:HE1	1.85	0.41
1:D:275:MET:HB3	1:D:276:PRO:HD3	2.03	0.41
1:D:317:ARG:H	1:D:317:ARG:CD	2.34	0.41
1:E:4:THR:O	1:E:4:THR:HG23	2.21	0.41
2:R:1:C:H2'	2:R:2:C:O4'	2.20	0.41
1:A:195:VAL:CG2	1:A:196:ALA:N	2.83	0.41
1:A:369:PRO:HA	1:A:370:PRO:HD3	1.80	0.41
1:B:81:ARG:HD2	1:B:208:HIS:NE2	2.33	0.41
1:B:160:LEU:HA	1:B:163:GLN:OE1	2.21	0.41
1:B:181:ILE:H	1:B:181:ILE:CD1	2.24	0.41
1:B:263:LEU:HD12	1:B:263:LEU:HA	1.88	0.41
1:C:200:MET:HB2	1:C:277:TYR:CE2	2.56	0.41
1:C:382:PHE:O	1:C:383:GLU:C	2.59	0.41
1:D:29:ALA:C	1:D:31:TYR:N	2.71	0.41
1:D:88:TRP:CD2	1:D:204:MET:HE3	2.56	0.41
1:E:38:ILE:CD1	1:E:107:LEU:O	2.69	0.41
1:A:151:GLU:HG2	1:A:155:LYS:HD3	2.02	0.41
1:A:160:LEU:HA	1:A:163:GLN:OE1	2.20	0.41
1:B:195:VAL:CG2	1:B:196:ALA:N	2.83	0.41
1:B:397:ALA:HB1	1:B:420:PHE:CG	2.55	0.41
1:D:153:ARG:HH12	1:D:177:GLU:HB2	1.86	0.41
1:D:248:TRP:O	1:D:250:LEU:HG	2.20	0.41
1:D:398:LYS:O	1:D:402:MET:HG2	2.20	0.41
1:B:31:TYR:C	1:B:33:ARG:N	2.74	0.41
1:B:233:HIS:HB2	1:B:312:ARG:NH1	2.35	0.41
1:C:68:HIS:CE1	1:C:118:PRO:HD2	2.56	0.41
1:C:160:LEU:HA	1:C:163:GLN:OE1	2.21	0.41
1:D:158:ASP:C	1:D:160:LEU:H	2.24	0.41
1:D:177:GLU:HG2	1:D:178:GLY:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:LYS:HB2	1:E:78:LYS:HE2	1.73	0.41
1:E:195:VAL:CG2	1:E:196:ALA:N	2.84	0.41
1:B:150:PRO:N	1:B:152:TYR:CE1	2.89	0.41
1:C:18:LEU:HD12	1:D:232:GLY:HA2	2.02	0.41
1:C:54:TYR:CD1	1:C:118:PRO:HB2	2.55	0.41
1:C:81:ARG:HD2	1:C:208:HIS:NE2	2.34	0.41
1:C:91:PHE:CE2	1:C:267:GLU:HG3	2.56	0.41
1:C:149:MET:C	1:C:152:TYR:CZ	2.94	0.41
1:D:149:MET:O	1:D:152:TYR:CG	2.74	0.41
1:D:303:LEU:CD2	1:D:328:THR:HA	2.51	0.41
1:E:81:ARG:HD2	1:E:208:HIS:NE2	2.34	0.41
1:E:397:ALA:HB1	1:E:420:PHE:CG	2.56	0.41
1:A:151:GLU:CD	2:R:33:C:H4'	2.40	0.41
1:A:255:ALA:O	1:A:259:VAL:HG23	2.20	0.41
1:A:354:LYS:CE	1:A:356:THR:HA	2.40	0.41
1:C:73:LEU:O	1:C:74:TYR:C	2.59	0.41
1:C:86:LYS:HB3	1:C:87:ASP:H	1.59	0.41
1:C:134:LEU:HD22	1:C:134:LEU:HA	1.95	0.41
1:C:153:ARG:CZ	1:C:176:PRO:HA	2.51	0.41
1:C:202:PHE:CG	1:C:211:ALA:HA	2.56	0.41
1:C:208:HIS:CE1	1:C:209:GLU:HG3	2.56	0.41
1:C:240:MET:HE3	1:C:244:ASP:HB3	2.03	0.41
1:C:366:THR:C	1:C:368:ALA:H	2.23	0.41
1:D:28:PRO:O	1:D:31:TYR:HB3	2.21	0.41
1:D:78:LYS:HE2	1:D:78:LYS:HB2	1.74	0.41
1:D:112:ALA:HB1	1:D:113:LEU:HD23	2.02	0.41
1:D:149:MET:C	1:D:152:TYR:CZ	2.94	0.41
1:E:208:HIS:CE1	1:E:210:CYS:HB2	2.56	0.41
1:E:295:PRO:HB2	1:E:322:ILE:HG21	2.03	0.41
1:A:81:ARG:HD2	1:A:208:HIS:NE2	2.35	0.41
1:A:361:THR:HB	1:A:362:GLY:H	1.77	0.41
1:B:215:TYR:C	1:B:215:TYR:CD2	2.94	0.41
1:C:123:ASP:C	1:C:125:SER:H	2.25	0.41
1:D:134:LEU:HD22	1:D:134:LEU:HA	1.96	0.41
1:A:55:VAL:O	1:A:56:TYR:C	2.57	0.40
1:A:303:LEU:CD2	1:A:328:THR:HA	2.51	0.40
1:B:14:ILE:CD1	1:C:259:VAL:HA	2.51	0.40
1:C:150:PRO:N	1:C:152:TYR:CZ	2.89	0.40
1:D:31:TYR:CD1	1:D:32:PHE:N	2.88	0.40
1:E:38:ILE:O	1:E:108:VAL:HB	2.20	0.40
1:E:53:GLY:O	1:E:54:TYR:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:MET:HE3	1:E:244:ASP:CB	2.51	0.40
1:A:155:LYS:NZ	2:R:35:C:OP2	2.43	0.40
1:A:397:ALA:HB1	1:A:420:PHE:CG	2.57	0.40
1:B:89:SER:O	1:B:90:SER:CB	2.65	0.40
1:C:58:GLY:O	1:C:63:ASN:O	2.39	0.40
1:C:382:PHE:CD2	1:C:387:ARG:HA	2.56	0.40
1:C:387:ARG:CZ	1:C:387:ARG:HB3	2.51	0.40
1:C:415:TYR:CD1	1:C:415:TYR:C	2.95	0.40
1:A:38:ILE:O	1:A:108:VAL:HB	2.20	0.40
1:A:308:LEU:HD12	1:A:308:LEU:HA	1.86	0.40
1:B:14:ILE:HD12	1:C:259:VAL:HG22	2.03	0.40
1:B:31:TYR:CD1	1:B:32:PHE:N	2.89	0.40
1:B:249:ILE:HD13	1:B:254:VAL:HG12	2.02	0.40
1:C:151:GLU:HG2	1:C:155:LYS:HD3	2.03	0.40
1:C:389:PRO:HB3	1:C:393:MET:HE3	2.03	0.40
1:D:66:ILE:HD13	1:D:185:TRP:CD1	2.56	0.40
1:D:382:PHE:HE1	1:D:393:MET:HE2	1.86	0.40
1:E:182:PHE:CD2	1:E:182:PHE:N	2.90	0.40
1:E:202:PHE:CG	1:E:211:ALA:HA	2.56	0.40
1:A:86:LYS:HB3	1:A:87:ASP:H	1.58	0.40
1:A:202:PHE:CG	1:A:211:ALA:HA	2.56	0.40
1:A:240:MET:HE3	1:A:244:ASP:CB	2.51	0.40
1:A:369:PRO:HB3	1:A:381:TRP:CZ2	2.56	0.40
1:A:421:ASP:O	1:A:422:LYS:HB3	2.20	0.40
1:C:88:TRP:CZ3	1:C:204:MET:HG2	2.57	0.40
1:C:93:ILE:N	1:C:93:ILE:HD12	2.37	0.40
1:E:66:ILE:HD13	1:E:185:TRP:CD1	2.57	0.40
1:E:153:ARG:HH12	1:E:177:GLU:HB2	1.87	0.40
1:E:215:TYR:CD1	2:R:45:C:H5"	2.56	0.40
1:A:38:ILE:CD1	1:A:107:LEU:O	2.70	0.40
1:A:354:LYS:NZ	1:E:380:GLY:HA2	2.37	0.40
1:A:397:ALA:O	1:A:401:VAL:HG22	2.21	0.40
1:B:119:ASP:OD1	1:B:119:ASP:N	2.55	0.40
1:B:151:GLU:HG2	1:B:155:LYS:HD3	2.03	0.40
1:B:253:GLU:CD	1:B:253:GLU:N	2.71	0.40
1:C:37:GLU:CB	1:C:108:VAL:HG11	2.43	0.40
1:C:74:TYR:O	1:C:78:LYS:HD3	2.20	0.40
1:D:309:ARG:HH11	1:D:309:ARG:HD3	1.78	0.40
1:E:79:ASP:O	1:E:79:ASP:CG	2.60	0.40
1:E:263:LEU:HD12	1:E:263:LEU:HA	1.91	0.40
1:E:410:LYS:NZ	2:R:40:C:N4	2.68	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	419/421 (100%)	306 (73%)	82 (20%)	31 (7%)	1	6
1	B	411/421 (98%)	302 (74%)	73 (18%)	36 (9%)	1	4
1	C	409/421 (97%)	296 (72%)	73 (18%)	40 (10%)	0	3
1	D	412/421 (98%)	303 (74%)	75 (18%)	34 (8%)	1	5
1	E	419/421 (100%)	303 (72%)	76 (18%)	40 (10%)	0	3
All	All	2070/2105 (98%)	1510 (73%)	379 (18%)	181 (9%)	1	4

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	44	THR
1	A	60	LYS
1	A	61	SER
1	A	79	ASP
1	A	90	SER
1	A	131	ASP
1	A	150	PRO
1	B	43	ASN
1	B	60	LYS
1	B	61	SER
1	B	79	ASP
1	B	90	SER
1	B	131	ASP
1	B	150	PRO
1	B	168	ASN
1	B	169	GLU
1	C	43	ASN

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Mol	Chain	Res	Type
1	C	60	LYS
1	C	79	ASP
1	C	90	SER
1	C	131	ASP
1	C	150	PRO
1	C	170	GLN
1	D	43	ASN
1	D	44	THR
1	D	60	LYS
1	D	61	SER
1	D	79	ASP
1	D	90	SER
1	D	131	ASP
1	D	271	ALA
1	E	43	ASN
1	E	60	LYS
1	E	61	SER
1	E	79	ASP
1	E	90	SER
1	E	131	ASP
1	E	150	PRO
1	E	271	ALA
1	E	360	SER
1	E	365	THR
1	A	4	THR
1	A	30	ASP
1	A	84	LEU
1	A	100	ASP
1	A	172	GLU
1	A	173	PRO
1	A	271	ALA
1	B	4	THR
1	B	30	ASP
1	B	44	THR
1	B	84	LEU
1	B	100	ASP
1	B	170	GLN
1	B	173	PRO
1	B	176	PRO
1	B	208	HIS
1	B	271	ALA
1	B	344	LEU

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Mol	Chain	Res	Type
1	C	4	THR
1	C	30	ASP
1	C	44	THR
1	C	61	SER
1	C	100	ASP
1	C	172	GLU
1	C	173	PRO
1	C	176	PRO
1	C	208	HIS
1	C	271	ALA
1	C	343	ASP
1	D	4	THR
1	D	30	ASP
1	D	84	LEU
1	D	100	ASP
1	D	150	PRO
1	D	171	PHE
1	D	172	GLU
1	D	173	PRO
1	D	176	PRO
1	D	208	HIS
1	E	4	THR
1	E	44	THR
1	E	84	LEU
1	E	100	ASP
1	E	164	CYS
1	E	168	ASN
1	E	172	GLU
1	E	173	PRO
1	E	208	HIS
1	A	28	PRO
1	A	81	ARG
1	A	112	ALA
1	A	117	LEU
1	A	129	ALA
1	A	176	PRO
1	A	177	GLU
1	A	208	HIS
1	A	343	ASP
1	A	344	LEU
1	B	63	ASN
1	B	81	ARG

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Mol	Chain	Res	Type
1	B	112	ALA
1	B	117	LEU
1	B	172	GLU
1	B	177	GLU
1	C	28	PRO
1	C	81	ARG
1	C	84	LEU
1	C	112	ALA
1	C	117	LEU
1	C	168	ASN
1	C	177	GLU
1	C	345	ALA
1	D	81	ARG
1	D	112	ALA
1	D	117	LEU
1	D	177	GLU
1	D	344	LEU
1	E	28	PRO
1	E	30	ASP
1	E	81	ARG
1	E	88	TRP
1	E	112	ALA
1	E	117	LEU
1	E	129	ALA
1	E	171	PHE
1	E	176	PRO
1	E	177	GLU
1	E	343	ASP
1	E	344	LEU
1	B	343	ASP
1	C	108	VAL
1	C	167	ILE
1	C	344	LEU
1	D	28	PRO
1	D	108	VAL
1	D	206	LYS
1	D	343	ASP
1	A	23	ASP
1	A	88	TRP
1	A	108	VAL
1	A	123	ASP
1	B	23	ASP

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Mol	Chain	Res	Type
1	B	28	PRO
1	B	88	TRP
1	B	108	VAL
1	B	123	ASP
1	C	23	ASP
1	C	88	TRP
1	C	129	ALA
1	C	206	LYS
1	C	228	LEU
1	D	23	ASP
1	D	63	ASN
1	D	88	TRP
1	D	123	ASP
1	D	167	ILE
1	E	23	ASP
1	E	108	VAL
1	E	123	ASP
1	E	363	GLY
1	E	364	LEU
1	A	206	LYS
1	B	239	GLY
1	C	63	ASN
1	C	123	ASP
1	C	174	LEU
1	D	106	ASP
1	E	174	LEU
1	C	239	GLY
1	B	219	VAL
1	B	16	PRO
1	C	16	PRO
1	C	219	VAL
1	D	219	VAL
1	A	16	PRO
1	B	19	PRO
1	E	167	ILE
1	E	219	VAL
1	E	16	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	362/362 (100%)	298 (82%)	64 (18%)	2	8
1	B	358/362 (99%)	293 (82%)	65 (18%)	1	7
1	C	356/362 (98%)	294 (83%)	62 (17%)	2	9
1	D	359/362 (99%)	296 (82%)	63 (18%)	2	8
1	E	362/362 (100%)	300 (83%)	62 (17%)	2	9
All	All	1797/1810 (99%)	1481 (82%)	316 (18%)	2	8

All (316) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	8	ILE
1	A	13	VAL
1	A	18	LEU
1	A	25	VAL
1	A	31	TYR
1	A	36	LYS
1	A	40	LEU
1	A	69	VAL
1	A	70	ASN
1	A	84	LEU
1	A	97	LYS
1	A	100	ASP
1	A	101	THR
1	A	117	LEU
1	A	119	ASP
1	A	123	ASP
1	A	126	ARG
1	A	134	LEU
1	A	148	GLN
1	A	152	TYR
1	A	153	ARG
1	A	156	LEU
1	A	160	LEU
1	A	162	ASN
1	A	169	GLU
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	172	GLU
1	A	174	LEU
1	A	175	VAL
1	A	180	ASP
1	A	181	ILE
1	A	183	ASP
1	A	187	ASN
1	A	209	GLU
1	A	217	THR
1	A	228	LEU
1	A	230	THR
1	A	241	SER
1	A	242	THR
1	A	243	GLU
1	A	252	ARG
1	A	253	GLU
1	A	268	ILE
1	A	291	SER
1	A	307	LEU
1	A	308	LEU
1	A	311	THR
1	A	317	ARG
1	A	325	THR
1	A	327	LEU
1	A	332	LEU
1	A	352	ASP
1	A	356	THR
1	A	358	ASP
1	A	359	ASP
1	A	361	THR
1	A	364	LEU
1	A	365	THR
1	A	384	ASP
1	A	385	GLN
1	A	405	GLN
1	A	410	LYS
1	A	414	LYS
1	B	3	VAL
1	B	8	ILE
1	B	13	VAL
1	B	18	LEU
1	B	25	VAL

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Mol	Chain	Res	Type
1	B	31	TYR
1	B	36	LYS
1	B	40	LEU
1	B	57	GLN
1	B	69	VAL
1	B	70	ASN
1	B	84	LEU
1	B	97	LYS
1	B	100	ASP
1	B	101	THR
1	B	107	LEU
1	B	117	LEU
1	B	119	ASP
1	B	123	ASP
1	B	126	ARG
1	B	134	LEU
1	B	148	GLN
1	B	152	TYR
1	B	153	ARG
1	B	156	LEU
1	B	160	LEU
1	B	162	ASN
1	B	169	GLU
1	B	170	GLN
1	B	172	GLU
1	B	174	LEU
1	B	175	VAL
1	B	180	ASP
1	B	181	ILE
1	B	183	ASP
1	B	187	ASN
1	B	209	GLU
1	B	217	THR
1	B	228	LEU
1	B	230	THR
1	B	241	SER
1	B	242	THR
1	B	243	GLU
1	B	252	ARG
1	B	253	GLU
1	B	268	ILE
1	B	291	SER

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Mol	Chain	Res	Type
1	B	307	LEU
1	B	308	LEU
1	B	311	THR
1	B	317	ARG
1	B	325	THR
1	B	327	LEU
1	B	332	LEU
1	B	352	ASP
1	B	354	LYS
1	B	356	THR
1	B	358	ASP
1	B	365	THR
1	B	366	THR
1	B	384	ASP
1	B	385	GLN
1	B	405	GLN
1	B	410	LYS
1	B	414	LYS
1	C	3	VAL
1	C	8	ILE
1	C	13	VAL
1	C	18	LEU
1	C	25	VAL
1	C	31	TYR
1	C	36	LYS
1	C	40	LEU
1	C	57	GLN
1	C	69	VAL
1	C	70	ASN
1	C	84	LEU
1	C	97	LYS
1	C	100	ASP
1	C	101	THR
1	C	107	LEU
1	C	117	LEU
1	C	119	ASP
1	C	123	ASP
1	C	126	ARG
1	C	134	LEU
1	C	148	GLN
1	C	152	TYR
1	C	153	ARG

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Mol	Chain	Res	Type
1	C	156	LEU
1	C	160	LEU
1	C	162	ASN
1	C	167	ILE
1	C	169	GLU
1	C	170	GLN
1	C	172	GLU
1	C	174	LEU
1	C	175	VAL
1	C	180	ASP
1	C	181	ILE
1	C	183	ASP
1	C	187	ASN
1	C	209	GLU
1	C	217	THR
1	C	228	LEU
1	C	230	THR
1	C	241	SER
1	C	242	THR
1	C	243	GLU
1	C	252	ARG
1	C	253	GLU
1	C	268	ILE
1	C	291	SER
1	C	308	LEU
1	C	311	THR
1	C	317	ARG
1	C	325	THR
1	C	327	LEU
1	C	332	LEU
1	C	352	ASP
1	C	353	ASN
1	C	356	THR
1	C	384	ASP
1	C	385	GLN
1	C	405	GLN
1	C	410	LYS
1	C	414	LYS
1	D	3	VAL
1	D	8	ILE
1	D	13	VAL
1	D	18	LEU

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Mol	Chain	Res	Type
1	D	25	VAL
1	D	31	TYR
1	D	36	LYS
1	D	40	LEU
1	D	57	GLN
1	D	69	VAL
1	D	70	ASN
1	D	84	LEU
1	D	97	LYS
1	D	100	ASP
1	D	101	THR
1	D	117	LEU
1	D	119	ASP
1	D	123	ASP
1	D	126	ARG
1	D	134	LEU
1	D	148	GLN
1	D	152	TYR
1	D	153	ARG
1	D	156	LEU
1	D	160	LEU
1	D	162	ASN
1	D	167	ILE
1	D	169	GLU
1	D	172	GLU
1	D	174	LEU
1	D	175	VAL
1	D	180	ASP
1	D	181	ILE
1	D	183	ASP
1	D	187	ASN
1	D	209	GLU
1	D	217	THR
1	D	228	LEU
1	D	230	THR
1	D	242	THR
1	D	243	GLU
1	D	252	ARG
1	D	253	GLU
1	D	268	ILE
1	D	291	SER
1	D	307	LEU

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Mol	Chain	Res	Type
1	D	308	LEU
1	D	311	THR
1	D	317	ARG
1	D	325	THR
1	D	327	LEU
1	D	332	LEU
1	D	352	ASP
1	D	353	ASN
1	D	354	LYS
1	D	356	THR
1	D	358	ASP
1	D	366	THR
1	D	384	ASP
1	D	385	GLN
1	D	405	GLN
1	D	410	LYS
1	D	414	LYS
1	E	8	ILE
1	E	13	VAL
1	E	18	LEU
1	E	25	VAL
1	E	31	TYR
1	E	36	LYS
1	E	40	LEU
1	E	57	GLN
1	E	69	VAL
1	E	70	ASN
1	E	84	LEU
1	E	97	LYS
1	E	100	ASP
1	E	101	THR
1	E	117	LEU
1	E	119	ASP
1	E	123	ASP
1	E	126	ARG
1	E	134	LEU
1	E	148	GLN
1	E	152	TYR
1	E	153	ARG
1	E	156	LEU
1	E	160	LEU
1	E	162	ASN

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Mol	Chain	Res	Type
1	E	172	GLU
1	E	174	LEU
1	E	175	VAL
1	E	180	ASP
1	E	181	ILE
1	E	183	ASP
1	E	187	ASN
1	E	209	GLU
1	E	217	THR
1	E	228	LEU
1	E	230	THR
1	E	242	THR
1	E	243	GLU
1	E	252	ARG
1	E	253	GLU
1	E	268	ILE
1	E	272	ASP
1	E	291	SER
1	E	308	LEU
1	E	311	THR
1	E	317	ARG
1	E	325	THR
1	E	327	LEU
1	E	332	LEU
1	E	352	ASP
1	E	353	ASN
1	E	354	LYS
1	E	356	THR
1	E	358	ASP
1	E	359	ASP
1	E	365	THR
1	E	366	THR
1	E	384	ASP
1	E	385	GLN
1	E	405	GLN
1	E	410	LYS
1	E	414	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN

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Mol	Chain	Res	Type
1	A	57	GLN
1	A	70	ASN
1	A	170	GLN
1	A	203	HIS
1	A	260	GLN
1	A	266	GLN
1	A	347	GLN
1	A	386	ASN
1	B	11	ASN
1	B	57	GLN
1	B	70	ASN
1	B	168	ASN
1	B	170	GLN
1	B	190	ASN
1	B	203	HIS
1	B	260	GLN
1	B	266	GLN
1	B	347	GLN
1	B	386	ASN
1	C	11	ASN
1	C	57	GLN
1	C	70	ASN
1	C	170	GLN
1	C	203	HIS
1	C	260	GLN
1	C	266	GLN
1	C	347	GLN
1	C	386	ASN
1	D	11	ASN
1	D	57	GLN
1	D	70	ASN
1	D	168	ASN
1	D	203	HIS
1	D	266	GLN
1	D	347	GLN
1	D	386	ASN
1	E	11	ASN
1	E	57	GLN
1	E	70	ASN
1	E	203	HIS
1	E	260	GLN
1	E	266	GLN

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Mol	Chain	Res	Type
1	E	347	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	44/45 (97%)	18 (40%)	2 (4%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	3	C
2	R	5	C
2	R	10	C
2	R	13	C
2	R	17	C
2	R	18	C
2	R	19	C
2	R	22	C
2	R	23	C
2	R	25	C
2	R	28	C
2	R	30	C
2	R	31	C
2	R	40	C
2	R	41	C
2	R	42	C
2	R	44	C
2	R	45	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	18	C
2	R	41	C

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 20 ligands modelled in this entry, 20 are modelled with single atom - 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	421/421 (100%)	0.27	32 (7%) 13 5	70, 102, 138, 158	0
1	B	415/421 (98%)	0.12	13 (3%) 49 26	71, 101, 137, 157	0
1	C	413/421 (98%)	0.23	22 (5%) 26 12	71, 101, 137, 158	0
1	D	416/421 (98%)	0.24	22 (5%) 26 12	71, 102, 137, 158	0
1	E	421/421 (100%)	0.34	35 (8%) 11 4	70, 102, 140, 163	0
2	R	45/45 (100%)	-0.03	0 100 100	97, 110, 120, 121	0
All	All	2131/2150 (99%)	0.24	124 (5%) 23 10	70, 102, 138, 163	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	16.9
1	E	2	SER	14.9
1	B	2	SER	9.9
1	C	2	SER	9.8
1	A	362	GLY	8.3
1	D	2	SER	7.6
1	A	361	THR	7.5
1	A	353	ASN	6.4
1	E	363	GLY	5.7
1	A	83	LYS	5.7
1	E	362	GLY	5.7
1	E	112	ALA	5.5
1	C	83	LYS	5.1
1	D	158	ASP	4.8
1	D	113	LEU	4.7
1	E	95	ILE	4.6
1	C	121	VAL	4.5
1	A	363	GLY	4.5
1	E	101	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	96	GLY	4.2
1	C	101	THR	4.2
1	C	353	ASN	4.1
1	D	166	MET	4.1
1	A	102	ILE	4.0
1	C	98	ALA	4.0
1	A	82	GLY	4.0
1	A	98	ALA	3.9
1	E	365	THR	3.8
1	E	98	ALA	3.7
1	E	62	GLY	3.6
1	A	122	SER	3.6
1	B	62	GLY	3.6
1	E	121	VAL	3.5
1	D	371	GLN	3.5
1	D	274	TYR	3.5
1	E	113	LEU	3.5
1	E	96	GLY	3.4
1	C	99	GLY	3.4
1	E	88	TRP	3.3
1	A	121	VAL	3.3
1	B	274	TYR	3.2
1	E	43	ASN	3.2
1	A	355	TYR	3.2
1	A	95	ILE	3.2
1	A	360	SER	3.1
1	E	158	ASP	3.1
1	A	85	ASP	3.1
1	D	346	GLN	3.0
1	A	365	THR	3.0
1	E	44	THR	3.0
1	A	96	GLY	3.0
1	E	361	THR	3.0
1	D	43	ASN	2.9
1	A	357	PRO	2.9
1	C	97	LYS	2.9
1	D	68	HIS	2.9
1	A	269	ASP	2.9
1	E	97	LYS	2.9
1	D	97	LYS	2.9
1	A	359	ASP	2.9
1	A	84	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	367	ASN	2.9
1	B	42	ILE	2.8
1	C	367	ASN	2.8
1	D	215	TYR	2.8
1	E	57	GLN	2.8
1	E	274	TYR	2.8
1	B	158	ASP	2.8
1	E	355	TYR	2.7
1	D	33	ARG	2.7
1	E	42	ILE	2.7
1	D	147	THR	2.7
1	B	118	PRO	2.7
1	C	216	GLY	2.6
1	A	99	GLY	2.6
1	A	148	GLN	2.6
1	C	95	ILE	2.6
1	C	84	LEU	2.6
1	C	82	GLY	2.6
1	E	118	PRO	2.5
1	B	112	ALA	2.5
1	D	353	ASN	2.5
1	D	112	ALA	2.5
1	C	215	TYR	2.5
1	A	62	GLY	2.5
1	E	216	GLY	2.5
1	B	113	LEU	2.4
1	A	101	THR	2.4
1	E	99	GLY	2.4
1	C	168	ASN	2.4
1	A	158	ASP	2.4
1	B	68	HIS	2.4
1	D	355	TYR	2.4
1	E	114	ASP	2.4
1	E	3	VAL	2.3
1	E	56	TYR	2.3
1	E	83	LYS	2.3
1	D	13	VAL	2.3
1	D	122	SER	2.3
1	C	355	TYR	2.3
1	B	172	GLU	2.3
1	D	367	ASN	2.3
1	A	364	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	33	ARG	2.2
1	E	63	ASN	2.2
1	A	356	THR	2.2
1	B	215	TYR	2.2
1	C	14	ILE	2.2
1	A	215	TYR	2.2
1	D	114	ASP	2.2
1	A	45	THR	2.2
1	B	88	TRP	2.1
1	C	148	GLN	2.1
1	D	102	ILE	2.1
1	E	207	LYS	2.1
1	D	27	TYR	2.1
1	E	109	SER	2.1
1	E	94	ASN	2.1
1	A	358	ASP	2.1
1	C	346	GLN	2.1
1	E	117	LEU	2.1
1	C	357	PRO	2.0
1	C	88	TRP	2.0
1	B	147	THR	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, 95^{th} 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	IUM	B	527	1/3	0.81	0.10	156,156,156,156	1
3	IUM	E	535	1/3	0.87	0.07	160,160,160,160	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IUM	D	530	1/3	0.92	0.08	166,166,166,166	1
3	IUM	B	524	1/3	0.92	0.09	165,165,165,165	1
3	IUM	D	531	1/3	0.94	0.10	156,156,156,156	1
3	IUM	A	523	1/3	0.95	0.12	175,175,175,175	1
3	IUM	A	521	1/3	0.95	0.10	132,132,132,132	1
3	IUM	E	533	1/3	0.97	0.11	132,132,132,132	1
3	IUM	B	525	1/3	0.97	0.09	134,134,134,134	1
3	IUM	C	528	1/3	0.98	0.10	136,136,136,136	1
3	IUM	C	529	1/3	0.98	0.13	136,136,136,136	0
3	IUM	R	539	1/3	0.98	0.14	112,112,112,112	1
3	IUM	R	536	1/3	0.99	0.14	130,130,130,130	0
3	IUM	R	537	1/3	0.99	0.15	122,122,122,122	1
3	IUM	R	538	1/3	0.99	0.13	126,126,126,126	0
3	IUM	E	534	1/3	0.99	0.17	132,132,132,132	0
3	IUM	A	522	1/3	1.00	0.14	129,129,129,129	0
3	IUM	D	532	1/3	1.00	0.15	125,125,125,125	0
3	IUM	B	526	1/3	1.00	0.16	125,125,125,125	0
3	IUM	R	540	1/3	1.00	0.16	126,126,126,126	1

6.5 Other polymers (i)

There are no such residues in this entry.