Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:46 AM GMT

PDB ID	:	3PTX
Title	:	Crystal Structure of a vesicular stomatitis virus nucleocapsid-polyA complex
Authors	:	Luo, M.; Green, T.J.; Rowse, M.
Deposited on	:	2010-12-03
Resolution	:	3.00 Å(reported)

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

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

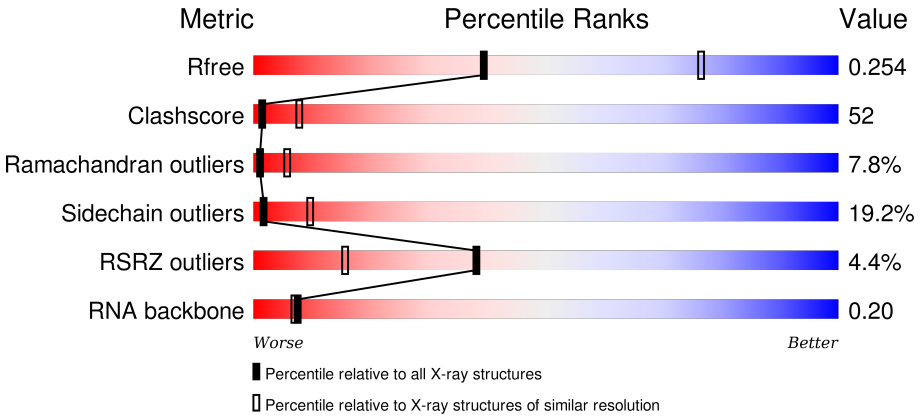
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5% 36% 47% 15% •
1	B	421	4% 33% 47% 16% ••
1	C	421	3% 33% 48% 16% ••
1	D	421	5% 34% 47% 16% ••

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Mol	Chain	Length	Quality of chain
1	E	421	5% 35% 47% 15%
2	R	45	7% 38% 51%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17527 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.

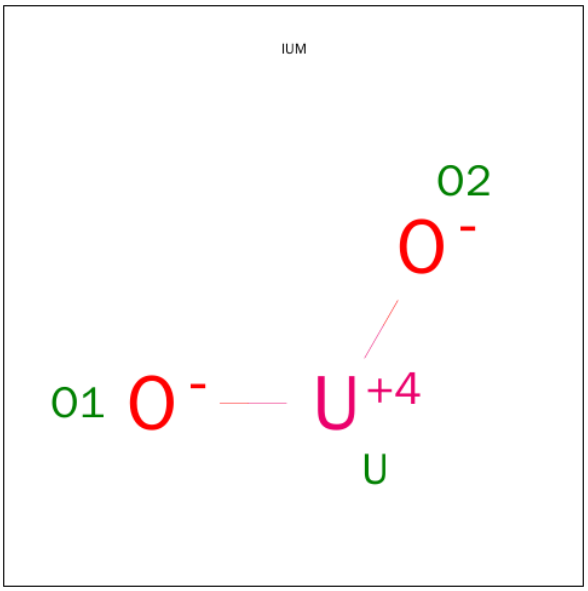
- Molecule 1 is a protein called Nucleoprotein.

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
			990	450	225	270	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	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	C	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	E	1	Total U 1 1	0	0
3	E	1	Total U 1 1	0	0

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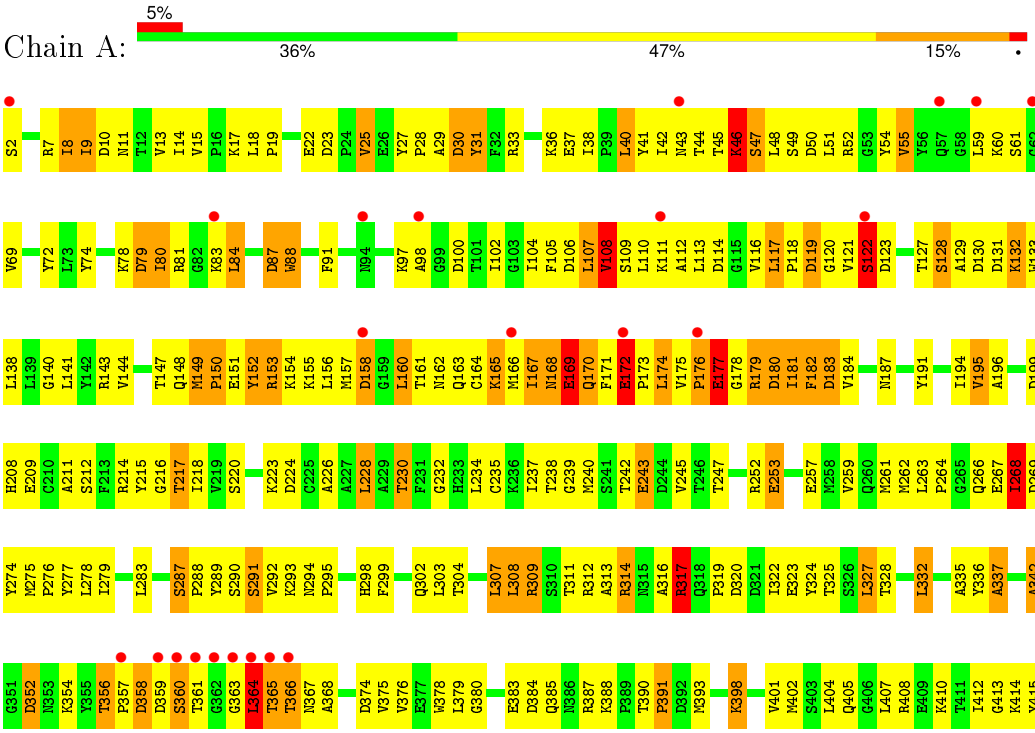
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0

3 Residue-property plots (i)

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

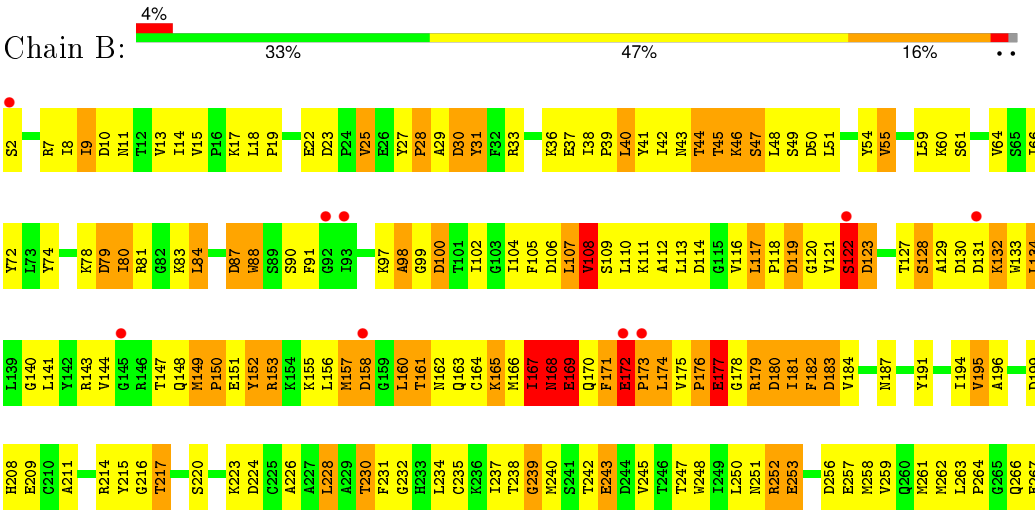
- Molecule 1: Nucleoprotein

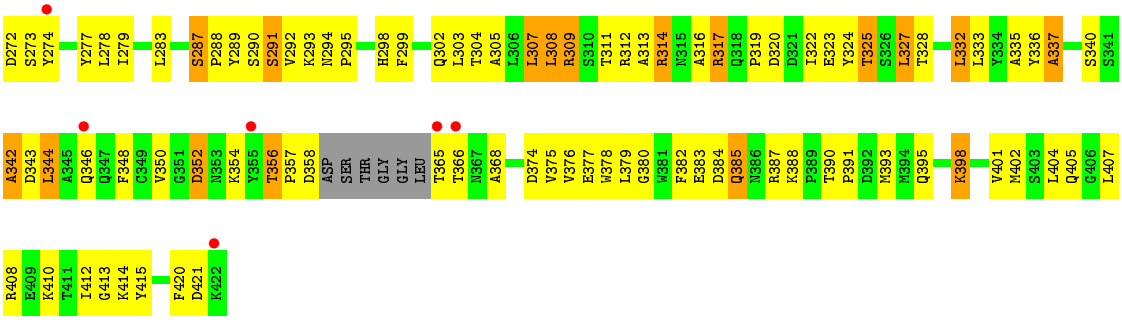
Chain A:



- Molecule 1: Nucleoprotein

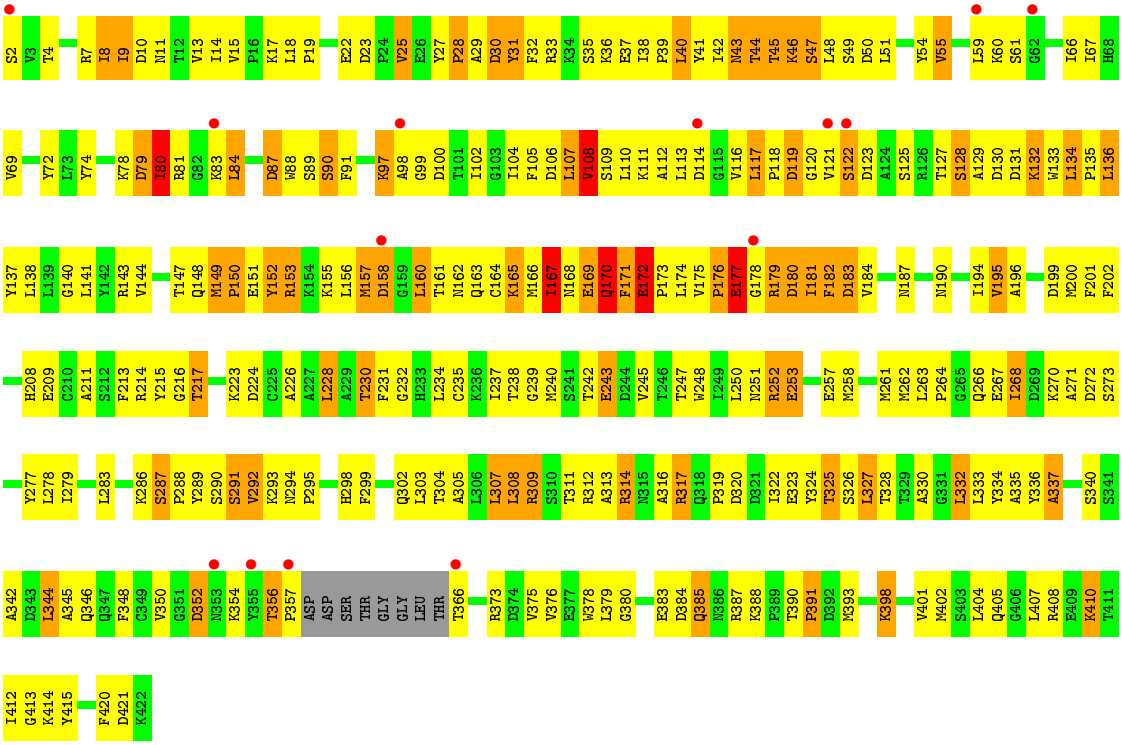
Chain B:





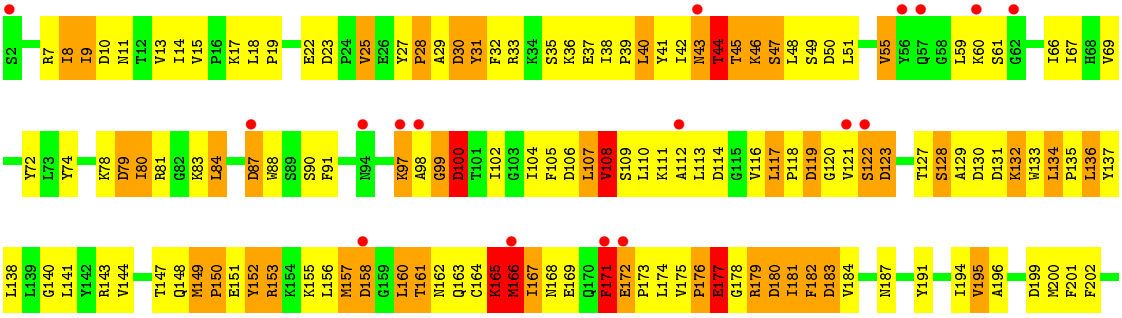
• Molecule 1: Nucleoprotein

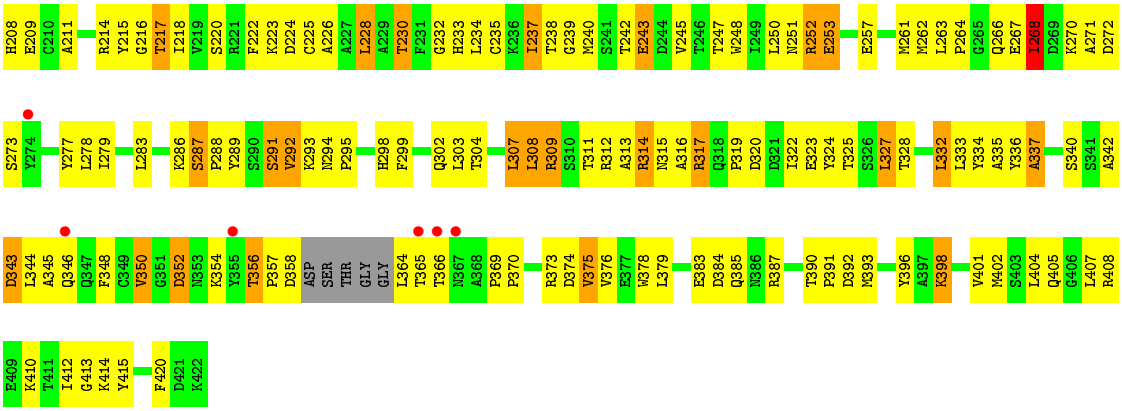
Chain C:



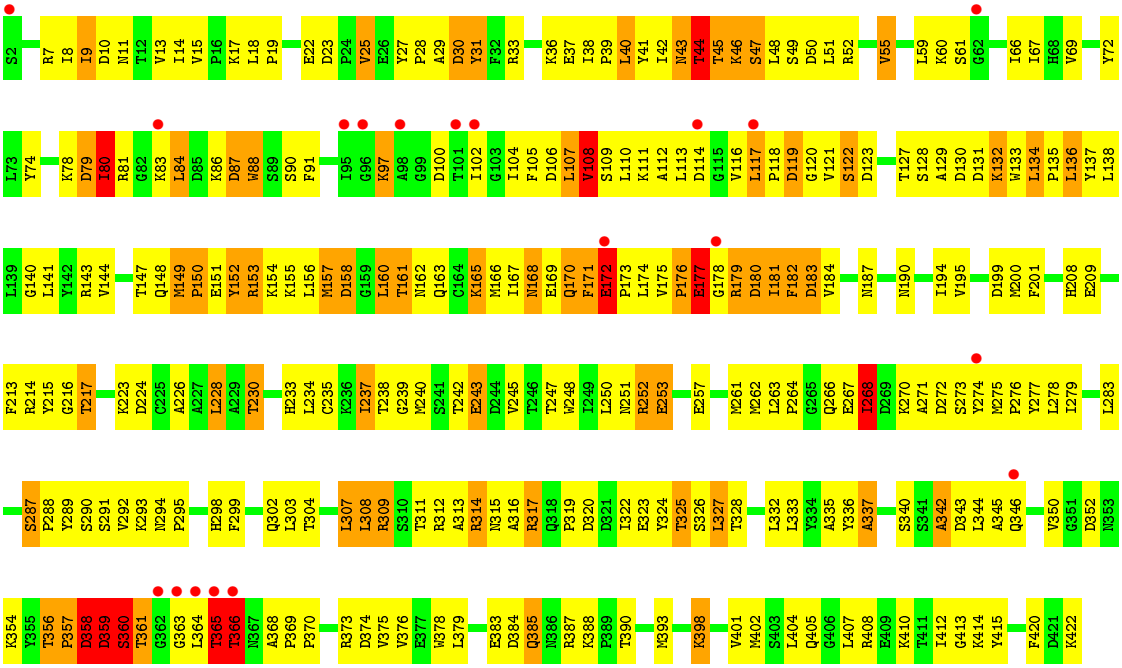
• Molecule 1: Nucleoprotein

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	166.41Å 233.61Å 73.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.96 – 3.00 40.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	76.8 (40.96-3.00) 76.9 (40.96-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.1_357)	Depositor
R, R_{free}	0.212 , 0.250 0.215 , 0.254	Depositor DCC
R_{free} test set	1885 reflections (4.17%)	DCC
Wilson B-factor (Å^2)	71.3	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 65.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 48095 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17527	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/3403	0.81	9/4607 (0.2%)
1	B	0.51	0/3365	0.81	13/4554 (0.3%)
1	C	0.51	0/3350	0.74	5/4533 (0.1%)
1	D	0.51	0/3373	0.71	3/4565 (0.1%)
1	E	0.51	0/3403	0.76	6/4607 (0.1%)
2	R	0.71	0/1124	1.17	2/1751 (0.1%)
All	All	0.53	0/18018	0.80	38/24617 (0.2%)

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	3
1	B	0	6
1	C	0	2
1	D	0	6
1	E	0	4
All	All	0	21

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	SER	N-CA-CB	-14.14	89.29	110.50
1	B	343	ASP	CB-CA-C	-11.87	86.67	110.40
1	A	122	SER	CB-CA-C	11.71	132.34	110.10
1	A	123	ASP	N-CA-CB	-11.58	89.76	110.60
1	B	168	ASN	N-CA-C	-9.14	86.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	358	ASP	N-CA-C	8.64	134.34	111.00
1	E	358	ASP	CB-CA-C	-8.48	93.43	110.40
1	E	8	ILE	N-CA-C	8.42	133.73	111.00
1	B	8	ILE	N-CA-C	8.36	133.58	111.00
1	B	343	ASP	N-CA-C	-8.36	88.43	111.00
1	A	8	ILE	N-CA-C	8.33	133.49	111.00
1	C	8	ILE	N-CA-C	8.31	133.43	111.00
1	A	344	LEU	N-CA-CB	-8.29	93.81	110.40
1	C	172	GLU	N-CA-CB	-8.14	95.94	110.60
1	C	172	GLU	N-CA-C	7.95	132.47	111.00
1	A	172	GLU	N-CA-CB	-7.79	96.58	110.60
1	A	172	GLU	N-CA-C	7.72	131.83	111.00
1	B	168	ASN	CB-CA-C	7.69	125.79	110.40
1	D	9	ILE	N-CA-CB	-7.47	93.61	110.80
1	E	9	ILE	N-CA-CB	-7.43	93.71	110.80
1	B	123	ASP	N-CA-CB	-7.33	97.41	110.60
1	B	9	ILE	N-CA-CB	-7.01	94.68	110.80
1	E	8	ILE	CB-CA-C	-7.00	97.61	111.60
1	C	9	ILE	N-CA-CB	-6.93	94.86	110.80
1	B	8	ILE	CB-CA-C	-6.88	97.84	111.60
1	A	9	ILE	N-CA-CB	-6.86	95.01	110.80
1	B	344	LEU	N-CA-CB	-6.51	97.39	110.40
1	B	171	PHE	CB-CA-C	-6.24	97.92	110.40
1	C	8	ILE	CB-CA-C	-6.19	99.21	111.60
1	B	167	ILE	N-CA-C	-6.17	94.33	111.00
1	D	166	MET	CB-CA-C	-6.17	98.06	110.40
1	A	8	ILE	CB-CA-C	-6.16	99.28	111.60
1	B	168	ASN	N-CA-CB	-5.93	99.92	110.60
1	E	358	ASP	C-N-CA	5.66	135.85	121.70
2	R	4	A	C3'-C2'-C1'	5.54	105.93	101.50
2	R	23	A	N1-C6-N6	5.22	121.73	118.60
1	B	169	GLU	N-CA-C	5.22	125.08	111.00
1	D	123	ASP	N-CA-CB	-5.06	101.49	110.60

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	SER	Peptide
1	A	169	GLU	Peptide
1	A	317	ARG	Sidechain
1	B	122	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	128	SER	Peptide
1	B	168	ASN	Peptide
1	B	170	GLN	Peptide
1	B	172	GLU	Peptide
1	B	173	PRO	Peptide
1	C	128	SER	Peptide
1	C	97	LYS	Peptide
1	D	128	SER	Peptide
1	D	165	LYS	Peptide
1	D	166	MET	Peptide
1	D	169	GLU	Peptide
1	D	171	PHE	Peptide
1	D	97	LYS	Peptide
1	E	357	PRO	Peptide
1	E	358	ASP	Peptide
1	E	359	ASP	Peptide
1	E	97	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3327	0	3287	354	0
1	B	3290	0	3253	381	0
1	C	3275	0	3242	366	0
1	D	3298	0	3264	365	0
1	E	3327	0	3287	345	0
2	R	990	0	496	147	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	R	5	0	0	0	0
All	All	17527	0	16829	1783	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 52.

All (1783) 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:B:172:GLU:HB3	1:B:173:PRO:CD	1.35	1.51
1:B:172:GLU:CB	1:B:173:PRO:HD3	1.52	1.32
1:D:317:ARG:NE	2:R:4:A:H2'	1.53	1.22
1:D:172:GLU:HB3	1:D:173:PRO:CD	1.67	1.21
1:D:317:ARG:HE	2:R:4:A:C2'	1.55	1.19
1:C:164:CYS:HA	1:C:168:ASN:HA	1.21	1.15
1:B:43:ASN:O	1:B:111:LYS:HE3	1.47	1.12
2:R:10:A:H4'	2:R:10:A:OP1	1.43	1.11
1:A:317:ARG:N	1:A:317:ARG:NH1	1.98	1.11
1:C:97:LYS:O	1:C:100:ASP:HB2	1.49	1.11
1:E:97:LYS:O	1:E:100:ASP:HB2	1.51	1.10
1:C:47:SER:HB3	1:C:50:ASP:HB2	1.33	1.10
1:D:8:ILE:HG13	1:D:9:ILE:H	1.11	1.09
1:E:133:TRP:CD1	1:E:167:ILE:HG21	1.88	1.08
1:D:47:SER:HB3	1:D:50:ASP:HB2	1.34	1.08
1:D:172:GLU:HB3	1:D:173:PRO:HD2	1.19	1.08
1:A:214:ARG:HA	1:A:217:THR:HG22	1.35	1.08
1:E:356:THR:HG23	1:E:357:PRO:HD3	1.35	1.07
1:B:47:SER:HB3	1:B:50:ASP:HB2	1.34	1.06
1:D:172:GLU:CB	1:D:173:PRO:CD	2.32	1.05
1:A:43:ASN:OD1	1:A:112:ALA:HB3	1.55	1.05
1:E:47:SER:HB3	1:E:50:ASP:HB2	1.38	1.05
1:D:172:GLU:CG	1:D:173:PRO:HD3	1.85	1.04
1:B:214:ARG:HA	1:B:217:THR:HG22	1.39	1.04
1:C:214:ARG:HA	1:C:217:THR:HG22	1.37	1.04
1:D:214:ARG:HA	1:D:217:THR:HG22	1.36	1.04
1:E:214:ARG:HA	1:E:217:THR:HG22	1.38	1.03
1:A:343:ASP:OD1	1:E:326:SER:HB3	1.58	1.01
1:A:226:ALA:HB2	2:R:31:A:H5"	1.43	1.01
1:B:84:LEU:O	1:B:99:GLY:HA2	1.57	1.01
1:D:129:ALA:HB1	1:D:167:ILE:HD13	1.42	1.00
2:R:4:A:H4'	2:R:5:A:OP1	1.58	1.00
1:D:317:ARG:HE	2:R:4:A:H2'	0.84	0.99
1:D:166:MET:O	1:D:167:ILE:HG13	1.63	0.99
1:D:163:GLN:O	1:D:166:MET:HB2	1.64	0.97
1:A:364:LEU:HD22	1:A:368:ALA:HB2	1.46	0.97
1:A:43:ASN:O	1:A:111:LYS:HE3	1.64	0.96
1:D:166:MET:O	1:D:167:ILE:CG1	2.14	0.96
1:D:84:LEU:O	1:D:99:GLY:HA2	1.64	0.96
1:A:226:ALA:HB2	2:R:31:A:C5'	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:10:A:H8	2:R:10:A:H5"	1.30	0.96
1:D:177:GLU:HA	1:D:181:ILE:HD11	1.47	0.95
1:A:117:LEU:HB2	1:A:118:PRO:HD3	1.49	0.95
1:B:177:GLU:HA	1:B:181:ILE:HD11	1.49	0.95
2:R:10:A:H5"	2:R:10:A:C8	2.01	0.94
1:C:177:GLU:HA	1:C:181:ILE:HD11	1.48	0.94
1:E:177:GLU:HA	1:E:181:ILE:HD11	1.48	0.94
1:D:226:ALA:O	1:D:230:THR:HG23	1.68	0.94
1:D:167:ILE:O	1:D:167:ILE:HG22	1.67	0.94
1:D:132:LYS:O	1:D:166:MET:SD	2.27	0.93
1:A:133:TRP:HD1	1:A:167:ILE:HG21	1.31	0.93
1:E:226:ALA:O	1:E:230:THR:HG23	1.69	0.92
1:E:150:PRO:HA	1:E:152:TYR:CE1	2.05	0.92
1:D:317:ARG:H	1:D:317:ARG:CZ	1.83	0.92
1:A:226:ALA:O	1:A:230:THR:HG23	1.69	0.92
1:C:117:LEU:HB2	1:C:118:PRO:HD3	1.50	0.92
1:E:117:LEU:HB2	1:E:118:PRO:HD3	1.52	0.91
1:A:177:GLU:HA	1:A:181:ILE:HD11	1.52	0.91
1:C:150:PRO:HA	1:C:152:TYR:CE1	2.06	0.90
1:D:117:LEU:HB2	1:D:118:PRO:HD3	1.52	0.90
1:B:184:VAL:HG11	1:C:166:MET:H	1.36	0.90
1:B:117:LEU:HB2	1:B:118:PRO:HD3	1.52	0.90
1:D:150:PRO:HA	1:D:152:TYR:CE1	2.07	0.90
2:R:6:A:H5"	2:R:7:A:O5'	1.72	0.90
1:A:150:PRO:HA	1:A:152:TYR:CE1	2.06	0.89
1:B:150:PRO:HA	1:B:152:TYR:CE1	2.08	0.89
1:A:356:THR:HG23	1:A:357:PRO:HD3	1.52	0.89
1:A:181:ILE:H	1:A:181:ILE:HD12	1.38	0.89
1:E:317:ARG:CZ	1:E:317:ARG:H	1.86	0.88
1:D:8:ILE:HG13	1:D:9:ILE:N	1.85	0.87
1:B:226:ALA:O	1:B:230:THR:HG23	1.74	0.87
1:D:180:ASP:O	1:D:180:ASP:OD2	1.92	0.87
1:A:317:ARG:CZ	1:A:317:ARG:H	1.88	0.87
1:C:43:ASN:O	1:C:111:LYS:HE3	1.75	0.87
1:B:43:ASN:OD1	1:B:112:ALA:HB3	1.73	0.87
1:A:133:TRP:CD1	1:A:167:ILE:HG21	2.11	0.86
1:B:298:HIS:CD2	1:B:317:ARG:NH1	2.43	0.86
1:B:230:THR:HG21	1:B:298:HIS:CE1	2.11	0.85
1:B:43:ASN:O	1:B:111:LYS:CE	2.23	0.85
1:C:226:ALA:O	1:C:230:THR:HG23	1.76	0.85
1:A:72:TYR:CE1	1:A:134:LEU:HD12	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLU:H	1:B:253:GLU:CD	1.79	0.85
1:A:44:THR:HG22	1:A:46:LYS:NZ	1.92	0.84
1:A:43:ASN:ND2	1:A:113:LEU:H	1.75	0.84
1:B:181:ILE:H	1:B:181:ILE:HD12	1.40	0.83
1:A:317:ARG:NH1	1:A:317:ARG:H	1.74	0.83
1:C:180:ASP:O	1:C:180:ASP:OD2	1.97	0.83
1:C:107:LEU:HD12	1:C:107:LEU:N	1.94	0.83
1:A:107:LEU:HD12	1:A:107:LEU:N	1.93	0.83
1:A:230:THR:HG21	1:A:298:HIS:CE1	2.14	0.82
1:A:226:ALA:CB	2:R:31:A:H5"	2.09	0.82
1:E:172:GLU:HB3	1:E:173:PRO:HD3	1.62	0.82
1:C:317:ARG:NH1	1:C:317:ARG:O	2.12	0.82
1:C:28:PRO:HD2	1:C:266:GLN:HE21	1.45	0.82
1:E:181:ILE:H	1:E:181:ILE:HD12	1.42	0.82
1:A:253:GLU:H	1:A:253:GLU:CD	1.82	0.82
1:B:180:ASP:OD2	1:B:180:ASP:O	1.98	0.81
1:E:72:TYR:CE1	1:E:134:LEU:HD12	2.14	0.81
1:C:181:ILE:HD12	1:C:181:ILE:H	1.44	0.81
1:C:18:LEU:HD12	1:D:232:GLY:HA2	1.62	0.81
1:D:72:TYR:CE1	1:D:134:LEU:HD12	2.15	0.81
1:B:167:ILE:O	1:B:168:ASN:CB	2.28	0.81
1:D:172:GLU:CB	1:D:173:PRO:HD3	2.03	0.81
1:B:18:LEU:HD12	1:C:232:GLY:HA2	1.61	0.81
1:A:128:SER:HA	1:A:130:ASP:HB2	1.61	0.81
1:D:163:GLN:HA	1:D:166:MET:HG3	1.60	0.81
1:B:72:TYR:CE1	1:B:134:LEU:HD12	2.16	0.81
1:B:107:LEU:N	1:B:107:LEU:HD12	1.96	0.81
1:C:172:GLU:HB3	1:C:173:PRO:HD3	1.63	0.81
1:D:9:ILE:HG23	1:D:10:ASP:H	1.45	0.80
1:E:9:ILE:HG23	1:E:10:ASP:H	1.45	0.80
1:D:107:LEU:HD12	1:D:107:LEU:N	1.97	0.80
1:B:9:ILE:HG23	1:B:10:ASP:H	1.46	0.80
1:D:253:GLU:H	1:D:253:GLU:CD	1.85	0.80
1:E:152:TYR:HD1	1:E:153:ARG:H	1.30	0.80
1:A:172:GLU:HB3	1:A:173:PRO:HD3	1.64	0.80
1:C:72:TYR:CE1	1:C:134:LEU:HD12	2.17	0.79
1:B:37:GLU:HB2	1:B:108:VAL:HG11	1.65	0.79
1:B:44:THR:HA	1:B:46:LYS:CE	2.12	0.79
2:R:24:A:H5"	2:R:25:A:OP1	1.82	0.79
1:D:230:THR:HG21	1:D:298:HIS:CE1	2.17	0.79
1:B:143:ARG:HH22	2:R:26:A:H3'	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:SER:HA	1:E:130:ASP:HB2	1.64	0.79
1:B:128:SER:HA	1:B:130:ASP:HB2	1.64	0.78
1:E:107:LEU:N	1:E:107:LEU:HD12	1.98	0.78
1:D:44:THR:HA	1:D:46:LYS:CE	2.14	0.78
1:C:230:THR:HG21	1:C:298:HIS:CE1	2.19	0.78
1:C:253:GLU:H	1:C:253:GLU:CD	1.85	0.78
1:D:148:GLN:O	1:D:152:TYR:HE2	1.65	0.78
1:C:164:CYS:CA	1:C:168:ASN:HA	2.10	0.78
1:A:43:ASN:HD21	1:A:113:LEU:H	1.27	0.78
1:A:45:THR:O	1:A:45:THR:HG22	1.83	0.78
1:E:44:THR:HA	1:E:46:LYS:CE	2.13	0.78
1:C:172:GLU:HB3	1:C:173:PRO:CD	2.14	0.77
1:A:172:GLU:HB3	1:A:173:PRO:CD	2.14	0.77
1:D:167:ILE:CG2	1:D:167:ILE:O	2.32	0.77
1:B:317:ARG:O	1:B:317:ARG:NH1	2.17	0.77
1:C:43:ASN:OD1	1:C:112:ALA:HB3	1.85	0.77
1:C:226:ALA:HB2	2:R:13:A:H5"	1.65	0.77
1:D:128:SER:HA	1:D:130:ASP:HB2	1.66	0.77
1:C:27:TYR:HB3	1:C:266:GLN:NE2	1.99	0.77
1:E:253:GLU:CD	1:E:253:GLU:H	1.87	0.77
1:D:153:ARG:CZ	1:D:176:PRO:HA	2.15	0.77
1:B:317:ARG:CZ	1:B:317:ARG:H	1.98	0.77
1:A:27:TYR:HB3	1:A:266:GLN:NE2	2.00	0.77
1:C:214:ARG:HA	1:C:217:THR:CG2	2.14	0.77
1:C:128:SER:HA	1:C:130:ASP:HB2	1.65	0.77
1:D:43:ASN:OD1	1:D:112:ALA:HB3	1.85	0.77
1:C:148:GLN:NE2	1:C:179:ARG:HE	1.83	0.76
1:E:230:THR:HG21	1:E:298:HIS:CE1	2.19	0.76
1:C:37:GLU:HB2	1:C:108:VAL:HG11	1.68	0.76
1:D:37:GLU:HB2	1:D:108:VAL:HG11	1.66	0.76
1:A:214:ARG:HA	1:A:217:THR:CG2	2.14	0.76
1:E:180:ASP:OD2	1:E:180:ASP:O	2.03	0.76
1:E:43:ASN:OD1	1:E:112:ALA:HB3	1.85	0.76
1:D:148:GLN:NE2	1:D:179:ARG:HE	1.82	0.76
1:C:148:GLN:O	1:C:152:TYR:HE2	1.68	0.76
1:A:9:ILE:HG23	1:A:10:ASP:H	1.50	0.76
1:B:383:GLU:HG3	1:C:354:LYS:HE2	1.68	0.76
1:D:214:ARG:HA	1:D:217:THR:CG2	2.15	0.76
1:E:172:GLU:HB3	1:E:173:PRO:CD	2.15	0.76
1:B:148:GLN:NE2	1:B:179:ARG:HE	1.84	0.76
1:D:153:ARG:NH2	1:D:176:PRO:HA	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LEU:HD13	1:D:344:LEU:HD12	1.66	0.75
1:E:153:ARG:CZ	1:E:176:PRO:HA	2.16	0.75
1:B:43:ASN:HD21	1:B:113:LEU:H	1.32	0.75
1:E:37:GLU:HB2	1:E:108:VAL:HG11	1.66	0.75
1:E:66:ILE:HD12	1:E:69:VAL:HG22	1.68	0.75
1:A:317:ARG:HH21	2:R:32:A:P	2.09	0.75
1:D:8:ILE:CG1	1:D:9:ILE:H	1.98	0.75
1:D:105:PHE:C	1:D:107:LEU:H	1.89	0.75
1:A:317:ARG:NH1	1:A:317:ARG:O	2.18	0.75
1:B:153:ARG:CZ	1:B:176:PRO:HA	2.17	0.74
1:B:214:ARG:HA	1:B:217:THR:CG2	2.16	0.74
1:A:180:ASP:OD2	1:A:180:ASP:O	2.05	0.74
1:C:44:THR:HA	1:C:46:LYS:CE	2.18	0.74
1:B:167:ILE:HG22	1:B:168:ASN:H	1.49	0.74
1:A:37:GLU:HB2	1:A:108:VAL:HG11	1.68	0.74
1:E:43:ASN:O	1:E:111:LYS:HE3	1.88	0.74
1:E:28:PRO:HD2	1:E:266:GLN:HE21	1.52	0.74
1:B:43:ASN:ND2	1:B:113:LEU:H	1.84	0.74
1:B:27:TYR:HB3	1:B:266:GLN:NE2	2.03	0.74
1:E:149:MET:O	1:E:151:GLU:N	2.21	0.74
1:E:149:MET:HG3	2:R:42:A:C1'	2.17	0.74
1:C:28:PRO:HD2	1:C:266:GLN:NE2	2.02	0.74
1:E:253:GLU:O	1:E:257:GLU:HG3	1.88	0.74
1:D:79:ASP:C	1:D:81:ARG:H	1.90	0.74
1:D:226:ALA:HB2	2:R:4:A:H5"	1.69	0.74
1:B:105:PHE:C	1:B:107:LEU:H	1.90	0.74
1:B:148:GLN:O	1:B:152:TYR:HE2	1.69	0.74
1:B:163:GLN:HB2	1:B:169:GLU:OE2	1.88	0.74
1:A:148:GLN:O	1:A:152:TYR:HE2	1.71	0.73
1:D:166:MET:O	1:D:167:ILE:CB	2.36	0.73
1:C:152:TYR:HD1	1:C:153:ARG:H	1.36	0.73
1:A:66:ILE:HD12	1:A:69:VAL:HG22	1.70	0.73
1:D:172:GLU:HG2	1:D:173:PRO:HD3	1.71	0.73
1:C:153:ARG:CZ	1:C:176:PRO:HA	2.18	0.73
1:C:9:ILE:HG23	1:C:10:ASP:H	1.50	0.73
1:A:149:MET:O	1:A:151:GLU:N	2.21	0.73
1:B:84:LEU:O	1:B:99:GLY:CA	2.34	0.73
1:A:44:THR:HG22	1:A:46:LYS:HZ3	1.52	0.73
1:D:42:ILE:HD12	1:D:74:TYR:HB2	1.70	0.73
1:E:148:GLN:NE2	1:E:179:ARG:HE	1.87	0.73
1:E:148:GLN:O	1:E:152:TYR:HE2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ARG:HA	1:E:217:THR:CG2	2.16	0.73
1:E:27:TYR:HB3	1:E:266:GLN:NE2	2.03	0.73
1:C:66:ILE:HD12	1:C:69:VAL:HG22	1.70	0.73
1:E:105:PHE:C	1:E:107:LEU:H	1.91	0.73
1:C:292:VAL:HG13	2:R:12:A:H5"	1.68	0.73
1:A:43:ASN:ND2	1:A:113:LEU:N	2.36	0.73
1:D:148:GLN:O	1:D:152:TYR:CE2	2.41	0.73
1:B:149:MET:O	1:B:151:GLU:N	2.22	0.73
1:E:317:ARG:NH2	2:R:41:A:OP2	2.22	0.73
1:D:129:ALA:CB	1:D:167:ILE:HD13	2.19	0.72
1:B:291:SER:HB3	2:R:22:A:OP2	1.88	0.72
1:B:40:LEU:HD22	1:B:42:ILE:HG13	1.70	0.72
1:B:152:TYR:HD1	1:B:153:ARG:H	1.37	0.72
1:D:66:ILE:HD12	1:D:69:VAL:HG22	1.70	0.72
1:D:179:ARG:HA	1:D:183:ASP:OD1	1.88	0.72
1:A:153:ARG:CZ	1:A:176:PRO:HA	2.18	0.72
1:C:140:GLY:HA2	1:C:216:GLY:HA3	1.69	0.72
1:A:152:TYR:HD1	1:A:153:ARG:H	1.38	0.72
1:B:179:ARG:HA	1:B:183:ASP:OD1	1.90	0.72
1:A:42:ILE:HD12	1:A:74:TYR:HB2	1.72	0.72
1:D:140:GLY:HA2	1:D:216:GLY:HA3	1.69	0.72
2:R:7:A:H4'	2:R:7:A:OP2	1.89	0.72
1:E:153:ARG:NH2	1:E:176:PRO:HA	2.04	0.72
1:A:46:LYS:H	1:A:46:LYS:HD2	1.55	0.72
1:D:152:TYR:HD1	1:D:153:ARG:H	1.37	0.72
1:C:149:MET:O	1:C:151:GLU:N	2.22	0.72
1:A:148:GLN:NE2	1:A:179:ARG:HE	1.87	0.72
1:D:317:ARG:N	1:D:317:ARG:CZ	2.53	0.71
2:R:43:A:OP2	2:R:43:A:H4'	1.87	0.71
1:B:317:ARG:NE	2:R:22:A:O2'	2.23	0.71
1:C:292:VAL:CG1	2:R:12:A:H5"	2.20	0.71
1:E:149:MET:HG3	2:R:42:A:H1'	1.70	0.71
1:E:179:ARG:HA	1:E:183:ASP:OD1	1.89	0.71
1:D:43:ASN:O	1:D:111:LYS:HE3	1.90	0.71
1:D:117:LEU:CB	1:D:118:PRO:HD3	2.21	0.71
1:B:167:ILE:O	1:B:168:ASN:HB2	1.89	0.71
1:E:165:LYS:O	1:E:167:ILE:HD12	1.91	0.71
1:C:79:ASP:C	1:C:81:ARG:H	1.93	0.71
1:D:171:PHE:CG	1:D:172:GLU:N	2.59	0.71
1:A:43:ASN:O	1:A:111:LYS:CE	2.38	0.71
1:B:140:GLY:HA2	1:B:216:GLY:HA3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:PRO:HD2	1:A:266:GLN:HE21	1.55	0.71
1:A:383:GLU:HG3	1:B:354:LYS:HE2	1.72	0.71
1:E:364:LEU:HB2	1:E:368:ALA:HB2	1.72	0.71
1:A:302:GLN:HG2	1:A:316:ALA:CB	2.20	0.71
1:A:317:ARG:C	1:A:317:ARG:HH11	1.93	0.71
1:C:179:ARG:HA	1:C:183:ASP:OD1	1.90	0.71
1:D:181:ILE:H	1:D:181:ILE:HD12	1.55	0.71
1:C:302:GLN:HG2	1:C:316:ALA:CB	2.20	0.71
1:B:28:PRO:HD2	1:B:266:GLN:HE21	1.56	0.71
1:A:79:ASP:C	1:A:81:ARG:H	1.92	0.71
1:C:167:ILE:O	1:C:169:GLU:CD	2.29	0.70
1:A:238:THR:C	1:A:240:MET:H	1.95	0.70
1:C:42:ILE:HD12	1:C:74:TYR:HB2	1.73	0.70
1:C:148:GLN:O	1:C:152:TYR:CE2	2.44	0.70
1:C:105:PHE:C	1:C:107:LEU:H	1.94	0.70
1:C:317:ARG:NH2	2:R:13:A:O2'	2.24	0.70
1:E:43:ASN:O	1:E:45:THR:N	2.24	0.70
1:C:376:VAL:HG21	1:D:352:ASP:OD1	1.91	0.70
1:A:179:ARG:HA	1:A:183:ASP:OD1	1.91	0.70
1:B:302:GLN:HG2	1:B:316:ALA:CB	2.21	0.70
1:B:66:ILE:HD12	1:B:69:VAL:HG22	1.74	0.70
1:E:140:GLY:HA2	1:E:216:GLY:HA3	1.73	0.70
1:C:165:LYS:O	1:C:167:ILE:HD13	1.92	0.70
1:B:298:HIS:HD2	1:B:317:ARG:NH1	1.87	0.70
1:E:150:PRO:CA	1:E:152:TYR:CE1	2.75	0.70
1:B:158:ASP:C	1:B:160:LEU:H	1.94	0.70
1:A:117:LEU:CB	1:A:118:PRO:HD3	2.20	0.70
1:C:165:LYS:O	1:C:167:ILE:CG1	2.39	0.70
1:B:18:LEU:CD1	1:C:232:GLY:HA2	2.22	0.69
1:D:51:LEU:O	1:D:55:VAL:HG22	1.92	0.69
1:A:376:VAL:HG21	1:B:352:ASP:OD1	1.91	0.69
1:B:79:ASP:C	1:B:81:ARG:H	1.93	0.69
1:B:153:ARG:NH2	1:B:176:PRO:HA	2.07	0.69
1:E:302:GLN:HG2	1:E:316:ALA:CB	2.22	0.69
1:C:224:ASP:HB2	1:C:279:ILE:HG13	1.73	0.69
1:E:153:ARG:NH1	1:E:176:PRO:O	2.25	0.69
2:R:10:A:H3'	2:R:11:A:H8	1.58	0.69
1:D:149:MET:O	1:D:151:GLU:N	2.26	0.69
1:A:153:ARG:NH2	1:A:176:PRO:HA	2.07	0.69
1:E:214:ARG:CA	1:E:217:THR:HG22	2.21	0.69
1:A:253:GLU:O	1:A:257:GLU:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:ASP:C	1:E:81:ARG:H	1.93	0.69
1:D:43:ASN:O	1:D:45:THR:N	2.25	0.69
1:B:51:LEU:O	1:B:55:VAL:HG22	1.92	0.69
1:E:224:ASP:HB2	1:E:279:ILE:HG13	1.74	0.69
1:E:160:LEU:HA	1:E:163:GLN:OE1	1.93	0.69
1:C:150:PRO:CA	1:C:152:TYR:CE1	2.75	0.69
1:A:105:PHE:C	1:A:107:LEU:H	1.94	0.68
1:E:42:ILE:HD12	1:E:74:TYR:HB2	1.75	0.68
1:A:140:GLY:HA2	1:A:216:GLY:HA3	1.73	0.68
1:A:51:LEU:O	1:A:55:VAL:HG22	1.93	0.68
1:B:148:GLN:O	1:B:152:TYR:CE2	2.45	0.68
1:C:117:LEU:CB	1:C:118:PRO:HD3	2.21	0.68
1:D:106:ASP:N	1:D:107:LEU:HD12	2.08	0.68
1:E:44:THR:CA	1:E:46:LYS:HD2	2.24	0.68
1:C:160:LEU:HA	1:C:163:GLN:OE1	1.93	0.68
1:C:379:LEU:HB3	1:D:354:LYS:HD3	1.74	0.68
1:B:152:TYR:HB3	1:B:177:GLU:OE2	1.94	0.68
1:B:117:LEU:CB	1:B:118:PRO:HD3	2.21	0.68
1:B:317:ARG:CZ	1:B:317:ARG:N	2.57	0.68
1:B:163:GLN:O	1:B:167:ILE:HB	1.94	0.68
1:B:44:THR:CA	1:B:46:LYS:HD2	2.23	0.68
1:C:153:ARG:NH2	1:C:176:PRO:HA	2.08	0.68
1:D:302:GLN:HG2	1:D:316:ALA:CB	2.23	0.68
1:B:122:SER:O	1:B:123:ASP:HB2	1.94	0.68
1:E:148:GLN:O	1:E:152:TYR:CE2	2.46	0.67
1:A:165:LYS:O	1:A:167:ILE:CD1	2.42	0.67
1:A:148:GLN:O	1:A:152:TYR:CE2	2.46	0.67
1:A:117:LEU:HB2	1:A:118:PRO:CD	2.23	0.67
1:C:238:THR:C	1:C:240:MET:H	1.97	0.67
1:A:43:ASN:OD1	1:A:112:ALA:CB	2.39	0.67
1:E:317:ARG:CZ	1:E:317:ARG:N	2.57	0.67
1:E:45:THR:HG22	1:E:45:THR:O	1.94	0.67
1:E:51:LEU:O	1:E:55:VAL:HG22	1.95	0.67
2:R:5:A:OP2	2:R:5:A:H8	1.76	0.67
1:C:18:LEU:CD1	1:D:232:GLY:HA2	2.24	0.67
1:B:18:LEU:HD12	1:C:232:GLY:CA	2.24	0.67
1:E:106:ASP:N	1:E:107:LEU:HD12	2.10	0.67
1:A:15:VAL:O	1:A:17:LYS:HG2	1.94	0.67
1:A:317:ARG:HH11	1:A:317:ARG:CA	2.08	0.67
1:A:106:ASP:N	1:A:107:LEU:HD12	2.09	0.67
1:A:150:PRO:CA	1:A:152:TYR:CE1	2.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ARG:NH1	1:B:176:PRO:O	2.28	0.67
1:A:165:LYS:O	1:A:167:ILE:HD12	1.93	0.67
1:E:117:LEU:CB	1:E:118:PRO:HD3	2.22	0.67
1:B:43:ASN:ND2	1:B:113:LEU:N	2.43	0.67
1:D:44:THR:CA	1:D:46:LYS:HD2	2.24	0.67
1:B:160:LEU:HA	1:B:163:GLN:OE1	1.94	0.67
1:E:28:PRO:HD2	1:E:266:GLN:NE2	2.10	0.67
1:D:263:LEU:HG	1:D:264:PRO:HD2	1.77	0.67
1:E:81:ARG:HB2	1:E:208:HIS:HE2	1.60	0.67
1:A:317:ARG:NH2	2:R:32:A:OP2	2.28	0.67
1:D:15:VAL:O	1:D:17:LYS:HG2	1.95	0.66
1:B:224:ASP:HB2	1:B:279:ILE:HG13	1.77	0.66
1:C:298:HIS:CD2	1:C:317:ARG:NH1	2.63	0.66
1:E:130:ASP:H	1:E:132:LYS:HG2	1.60	0.66
1:D:27:TYR:HB3	1:D:266:GLN:NE2	2.10	0.66
1:E:149:MET:C	1:E:152:TYR:CZ	2.68	0.66
1:A:160:LEU:HA	1:A:163:GLN:OE1	1.95	0.66
1:E:263:LEU:HG	1:E:264:PRO:HD2	1.78	0.66
1:D:44:THR:CG2	1:D:116:VAL:HG11	2.26	0.66
1:E:238:THR:C	1:E:240:MET:H	1.99	0.66
1:B:150:PRO:CA	1:B:152:TYR:CE1	2.79	0.66
1:A:153:ARG:NH1	1:A:176:PRO:O	2.28	0.66
1:A:263:LEU:HG	1:A:264:PRO:HD2	1.78	0.66
1:C:149:MET:C	1:C:152:TYR:CZ	2.69	0.66
1:D:387:ARG:NH1	1:D:387:ARG:HB3	2.11	0.66
1:A:224:ASP:HB2	1:A:279:ILE:HG13	1.76	0.65
1:C:106:ASP:N	1:C:107:LEU:HD12	2.10	0.65
1:D:149:MET:C	1:D:152:TYR:CZ	2.69	0.65
1:A:214:ARG:CA	1:A:217:THR:HG22	2.20	0.65
1:D:150:PRO:CA	1:D:152:TYR:CE1	2.78	0.65
1:A:317:ARG:NH1	1:A:317:ARG:CA	2.59	0.65
1:A:317:ARG:NH2	2:R:32:A:P	2.69	0.65
1:B:44:THR:CG2	1:B:116:VAL:HG11	2.27	0.65
1:D:214:ARG:CA	1:D:217:THR:HG22	2.20	0.65
1:A:158:ASP:C	1:A:160:LEU:H	1.99	0.65
1:E:387:ARG:NH1	1:E:387:ARG:HB3	2.10	0.65
1:C:238:THR:O	1:C:240:MET:N	2.29	0.65
1:B:385:GLN:HG2	1:B:390:THR:HG22	1.77	0.65
1:D:152:TYR:HB3	1:D:177:GLU:OE2	1.96	0.65
2:R:10:A:H3'	2:R:11:A:C8	2.32	0.65
2:R:30:A:H2'	2:R:31:A:O4'	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ASP:H	1:D:132:LYS:HG2	1.62	0.65
1:E:152:TYR:HB3	1:E:177:GLU:OE2	1.97	0.65
1:C:387:ARG:HB3	1:C:387:ARG:NH1	2.12	0.65
1:D:171:PHE:CD2	1:D:171:PHE:C	2.69	0.65
1:D:172:GLU:HB3	1:D:173:PRO:HD3	1.64	0.65
1:D:160:LEU:HA	1:D:163:GLN:OE1	1.96	0.65
1:D:98:ALA:O	1:D:100:ASP:N	2.30	0.65
1:E:9:ILE:HG23	1:E:10:ASP:N	2.10	0.65
1:D:238:THR:C	1:D:240:MET:H	2.00	0.65
1:A:152:TYR:HB3	1:A:177:GLU:OE2	1.97	0.65
1:E:44:THR:CG2	1:E:116:VAL:HG11	2.27	0.65
1:B:143:ARG:NH2	2:R:26:A:H3'	2.12	0.65
1:D:45:THR:O	1:D:45:THR:HG22	1.96	0.65
1:B:356:THR:HG23	1:B:357:PRO:HD3	1.77	0.65
1:B:408:ARG:HD3	2:R:24:A:C6	2.31	0.65
1:A:230:THR:HB	1:A:302:GLN:OE1	1.98	0.64
2:R:32:A:H5"	2:R:33:A:P	2.37	0.64
1:E:158:ASP:C	1:E:160:LEU:H	1.99	0.64
1:C:117:LEU:HB2	1:C:118:PRO:CD	2.24	0.64
1:B:376:VAL:HG21	1:C:352:ASP:OD1	1.97	0.64
1:D:117:LEU:HB2	1:D:118:PRO:CD	2.26	0.64
1:B:106:ASP:N	1:B:107:LEU:HD12	2.12	0.64
1:D:28:PRO:HD2	1:D:266:GLN:HE21	1.62	0.64
1:C:15:VAL:O	1:C:17:LYS:HG2	1.97	0.64
1:E:117:LEU:HB2	1:E:118:PRO:CD	2.26	0.64
1:C:51:LEU:O	1:C:55:VAL:HG22	1.98	0.64
1:D:224:ASP:HB2	1:D:279:ILE:HG13	1.79	0.64
1:D:278:LEU:HA	1:D:283:LEU:HD12	1.78	0.64
1:C:44:THR:CA	1:C:46:LYS:HD2	2.26	0.64
2:R:23:A:C2	2:R:25:A:H1'	2.33	0.64
1:D:172:GLU:HG3	1:D:173:PRO:HD3	1.76	0.64
1:C:130:ASP:H	1:C:132:LYS:HG2	1.63	0.64
1:B:379:LEU:HB3	1:C:354:LYS:HD3	1.79	0.64
1:E:385:GLN:HG2	1:E:390:THR:HG22	1.80	0.64
1:A:184:VAL:CG1	1:B:166:MET:HG2	2.27	0.64
1:D:365:THR:HG23	1:D:366:THR:HG22	1.80	0.64
1:D:158:ASP:C	1:D:160:LEU:H	2.00	0.64
1:C:302:GLN:HG2	1:C:316:ALA:HB2	1.80	0.64
1:C:18:LEU:HD12	1:D:232:GLY:CA	2.26	0.64
1:A:385:GLN:HG2	1:A:390:THR:HG22	1.79	0.64
2:R:15:A:H5"	2:R:16:A:O5'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:HIS:CD2	1:E:317:ARG:NH1	2.66	0.64
1:C:165:LYS:O	1:C:167:ILE:HG12	1.98	0.64
1:A:343:ASP:OD1	1:E:326:SER:CB	2.40	0.64
1:E:153:ARG:O	1:E:157:MET:HB2	1.97	0.64
1:C:356:THR:HG23	1:C:357:PRO:HD3	1.78	0.64
1:B:28:PRO:HD2	1:B:266:GLN:NE2	2.12	0.64
1:B:81:ARG:HB2	1:B:208:HIS:HE2	1.62	0.64
1:B:238:THR:C	1:B:240:MET:H	2.00	0.64
1:A:298:HIS:NE2	1:A:317:ARG:NH2	2.45	0.64
1:B:45:THR:HG22	1:B:45:THR:O	1.98	0.64
1:A:28:PRO:HD2	1:A:266:GLN:NE2	2.13	0.64
1:D:356:THR:HG23	1:D:357:PRO:HD3	1.79	0.64
1:A:359:ASP:O	1:A:361:THR:N	2.28	0.63
1:D:9:ILE:HG23	1:D:10:ASP:N	2.12	0.63
1:D:29:ALA:C	1:D:31:TYR:H	2.01	0.63
1:B:230:THR:HB	1:B:302:GLN:OE1	1.98	0.63
1:A:302:GLN:HG2	1:A:316:ALA:HB2	1.81	0.63
1:C:153:ARG:NH1	1:C:176:PRO:O	2.32	0.63
1:B:44:THR:HA	1:B:46:LYS:CD	2.29	0.63
1:B:263:LEU:HG	1:B:264:PRO:HD2	1.81	0.63
1:C:385:GLN:HG2	1:C:390:THR:HG22	1.79	0.63
1:C:153:ARG:O	1:C:157:MET:HB2	1.98	0.63
1:B:117:LEU:HB2	1:B:118:PRO:CD	2.25	0.63
1:D:153:ARG:O	1:D:157:MET:HB2	1.99	0.63
1:C:44:THR:CG2	1:C:116:VAL:HG11	2.29	0.63
1:C:317:ARG:CZ	1:C:317:ARG:H	2.12	0.63
1:A:291:SER:HB3	2:R:31:A:OP2	1.99	0.62
1:D:8:ILE:O	1:D:11:ASN:N	2.32	0.62
1:C:45:THR:O	1:C:45:THR:HG22	1.97	0.62
1:B:253:GLU:O	1:B:257:GLU:HG3	1.99	0.62
1:B:149:MET:C	1:B:152:TYR:CZ	2.72	0.62
1:A:130:ASP:H	1:A:132:LYS:HG2	1.64	0.62
1:D:81:ARG:HB2	1:D:208:HIS:HE2	1.64	0.62
1:C:163:GLN:O	1:C:167:ILE:HG13	1.99	0.62
1:B:387:ARG:HB3	1:B:387:ARG:NH1	2.14	0.62
1:A:238:THR:O	1:A:240:MET:N	2.31	0.62
1:A:153:ARG:O	1:A:157:MET:HB2	2.00	0.62
1:E:356:THR:CG2	1:E:357:PRO:HD3	2.23	0.62
1:B:184:VAL:HG11	1:C:166:MET:N	2.11	0.62
1:E:29:ALA:C	1:E:31:TYR:H	2.02	0.62
1:C:263:LEU:HG	1:C:264:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:HA	1:A:324:TYR:OH	2.00	0.62
1:D:44:THR:HA	1:D:46:LYS:CD	2.29	0.62
1:E:230:THR:HB	1:E:302:GLN:OE1	2.00	0.62
1:C:81:ARG:HB2	1:C:208:HIS:HE2	1.63	0.62
1:C:152:TYR:HB3	1:C:177:GLU:OE2	1.98	0.62
1:A:29:ALA:C	1:A:31:TYR:H	2.02	0.62
1:C:165:LYS:O	1:C:167:ILE:CD1	2.47	0.62
1:A:54:TYR:HD1	1:A:122:SER:HB2	1.64	0.62
1:E:15:VAL:O	1:E:17:LYS:HG2	2.00	0.62
1:E:171:PHE:CG	1:E:172:GLU:N	2.67	0.62
1:A:81:ARG:HB2	1:A:208:HIS:HE2	1.63	0.62
1:A:54:TYR:CD1	1:A:122:SER:HB2	2.35	0.62
1:D:137:TYR:CE2	1:D:141:LEU:HD11	2.34	0.62
1:C:253:GLU:O	1:C:257:GLU:HG3	2.00	0.62
1:B:144:VAL:O	1:B:147:THR:HG22	2.00	0.62
1:E:102:ILE:HB	1:E:106:ASP:OD2	2.00	0.62
1:A:387:ARG:NH1	1:A:387:ARG:HB3	2.14	0.62
1:E:238:THR:O	1:E:240:MET:N	2.32	0.62
1:D:385:GLN:HG2	1:D:390:THR:HG22	1.80	0.62
1:B:15:VAL:O	1:B:17:LYS:HG2	1.99	0.61
1:E:359:ASP:O	1:E:361:THR:N	2.33	0.61
1:E:44:THR:HA	1:E:46:LYS:CD	2.29	0.61
1:C:29:ALA:C	1:C:31:TYR:H	2.02	0.61
1:D:25:VAL:HG11	1:D:288:PRO:HA	1.82	0.61
1:D:44:THR:HG21	1:D:116:VAL:HG11	1.82	0.61
1:C:214:ARG:CA	1:C:217:THR:HG22	2.21	0.61
1:C:43:ASN:O	1:C:45:THR:N	2.33	0.61
1:C:230:THR:HB	1:C:302:GLN:OE1	2.00	0.61
1:A:379:LEU:HB3	1:B:354:LYS:HD3	1.81	0.61
1:D:172:GLU:CG	1:D:173:PRO:CD	2.65	0.61
1:A:149:MET:C	1:A:151:GLU:H	2.04	0.61
1:B:153:ARG:O	1:B:157:MET:HB2	2.00	0.61
1:C:29:ALA:O	1:C:31:TYR:N	2.34	0.61
1:B:29:ALA:C	1:B:31:TYR:H	2.02	0.61
1:A:18:LEU:HD12	1:B:232:GLY:HA2	1.81	0.61
1:D:317:ARG:O	1:D:319:PRO:HD3	2.00	0.61
1:B:214:ARG:CA	1:B:217:THR:HG22	2.22	0.61
1:B:317:ARG:O	1:B:319:PRO:HD3	2.00	0.61
1:D:253:GLU:O	1:D:257:GLU:HG3	2.00	0.61
1:A:166:MET:H	1:E:184:VAL:HG11	1.65	0.61
1:C:320:ASP:HA	1:C:324:TYR:OH	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:O	1:A:169:GLU:HG2	2.00	0.61
1:B:130:ASP:H	1:B:132:LYS:HG2	1.65	0.61
2:R:31:A:H8	2:R:31:A:OP2	1.84	0.61
1:B:97:LYS:O	1:B:100:ASP:HB2	2.00	0.61
1:B:302:GLN:HG2	1:B:316:ALA:HB2	1.83	0.61
1:B:29:ALA:O	1:B:31:TYR:N	2.34	0.61
1:A:165:LYS:C	1:A:167:ILE:H	2.03	0.61
1:C:158:ASP:C	1:C:160:LEU:H	2.01	0.60
1:E:137:TYR:CE2	1:E:141:LEU:HD11	2.35	0.60
1:C:149:MET:C	1:C:151:GLU:H	2.04	0.60
1:D:153:ARG:NH1	1:D:176:PRO:O	2.34	0.60
1:E:278:LEU:HA	1:E:283:LEU:HD12	1.82	0.60
1:E:25:VAL:HG11	1:E:288:PRO:HA	1.83	0.60
1:E:67:ILE:H	1:E:67:ILE:HD12	1.65	0.60
1:E:44:THR:HG21	1:E:116:VAL:HG11	1.83	0.60
1:E:44:THR:HA	1:E:46:LYS:NZ	2.17	0.60
1:E:320:ASP:HA	1:E:324:TYR:OH	2.02	0.60
1:D:320:ASP:HA	1:D:324:TYR:OH	2.01	0.60
1:D:175:VAL:HG13	1:D:181:ILE:HG12	1.82	0.60
1:D:230:THR:HB	1:D:302:GLN:OE1	2.02	0.60
1:B:328:THR:CG2	1:B:415:TYR:HE1	2.15	0.60
1:D:408:ARG:HD3	2:R:6:A:C6	2.37	0.60
1:C:44:THR:HA	1:C:46:LYS:CD	2.32	0.60
1:E:199:ASP:OD1	1:E:217:THR:HG23	2.02	0.60
1:E:364:LEU:C	1:E:366:THR:H	2.05	0.60
1:B:25:VAL:HG11	1:B:288:PRO:HA	1.84	0.60
1:A:149:MET:C	1:A:152:TYR:CZ	2.74	0.60
1:E:149:MET:C	1:E:151:GLU:H	2.05	0.60
1:D:180:ASP:C	1:D:180:ASP:OD2	2.39	0.60
1:A:44:THR:HG21	1:A:116:VAL:HG11	1.83	0.60
1:C:294:ASN:N	1:C:295:PRO:HD3	2.16	0.60
1:C:165:LYS:C	1:C:167:ILE:N	2.53	0.60
1:A:259:VAL:HG21	1:E:7:ARG:NH1	2.16	0.60
1:B:149:MET:C	1:B:151:GLU:H	2.05	0.60
1:B:9:ILE:HG23	1:B:10:ASP:N	2.15	0.60
1:C:328:THR:CG2	1:C:415:TYR:HE1	2.14	0.60
1:D:166:MET:O	1:D:167:ILE:HB	2.01	0.60
1:A:102:ILE:HB	1:A:106:ASP:OD2	2.02	0.60
1:D:43:ASN:HD21	1:D:113:LEU:H	1.49	0.60
1:B:238:THR:O	1:B:240:MET:N	2.35	0.60
1:D:29:ALA:O	1:D:31:TYR:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD13	1:A:393:MET:HE2	1.83	0.60
1:E:358:ASP:CG	1:E:359:ASP:H	2.04	0.59
1:E:302:GLN:HG2	1:E:316:ALA:HB2	1.83	0.59
1:C:102:ILE:HB	1:C:106:ASP:OD2	2.01	0.59
1:D:292:VAL:CG1	2:R:3:A:H5"	2.32	0.59
1:E:44:THR:HA	1:E:46:LYS:HZ2	1.67	0.59
1:D:294:ASN:N	1:D:295:PRO:HD3	2.17	0.59
1:C:59:LEU:C	1:C:61:SER:H	2.05	0.59
1:A:43:ASN:CG	1:A:112:ALA:HB3	2.22	0.59
1:D:328:THR:HG21	1:D:415:TYR:OH	2.02	0.59
1:A:25:VAL:HG11	1:A:288:PRO:HA	1.85	0.59
1:A:144:VAL:O	1:A:147:THR:HG22	2.02	0.59
1:D:238:THR:O	1:D:240:MET:N	2.36	0.59
1:B:44:THR:HG21	1:B:116:VAL:HG11	1.83	0.59
1:E:328:THR:HG21	1:E:415:TYR:OH	2.03	0.59
1:B:320:ASP:HA	1:B:324:TYR:OH	2.02	0.59
1:C:13:VAL:HG12	1:C:14:ILE:N	2.18	0.59
1:A:97:LYS:O	1:A:100:ASP:HB2	2.01	0.59
1:C:163:GLN:N	1:C:163:GLN:OE1	2.35	0.59
1:E:278:LEU:HD23	1:E:279:ILE:H	1.67	0.59
1:A:328:THR:CG2	1:A:415:TYR:HE1	2.16	0.59
1:B:294:ASN:N	1:B:295:PRO:HD3	2.18	0.59
1:E:317:ARG:O	1:E:319:PRO:HD3	2.03	0.58
1:E:165:LYS:O	1:E:167:ILE:CD1	2.51	0.58
1:C:175:VAL:HG13	1:C:181:ILE:HG12	1.83	0.58
1:E:175:VAL:HG13	1:E:181:ILE:HG12	1.85	0.58
1:B:385:GLN:HG2	1:B:390:THR:CG2	2.34	0.58
1:E:343:ASP:OD1	1:E:373:ARG:NH1	2.36	0.58
1:A:137:TYR:CE2	1:A:141:LEU:HD11	2.38	0.58
1:E:357:PRO:HA	1:E:360:SER:HB2	1.84	0.58
1:C:332:LEU:HD13	1:C:393:MET:HE2	1.84	0.58
1:A:67:ILE:H	1:A:67:ILE:HD12	1.68	0.58
1:D:160:LEU:O	1:D:160:LEU:HD12	2.03	0.58
1:E:149:MET:CG	2:R:42:A:H1'	2.33	0.58
1:E:226:ALA:HB2	2:R:40:A:OP1	2.03	0.58
1:A:9:ILE:HG23	1:A:10:ASP:N	2.16	0.58
1:D:298:HIS:CD2	1:D:317:ARG:NH1	2.71	0.58
1:A:317:ARG:O	1:A:319:PRO:HD3	2.02	0.58
1:A:44:THR:CG2	1:A:116:VAL:HG11	2.34	0.58
1:D:149:MET:O	1:D:152:TYR:CG	2.56	0.58
1:C:278:LEU:HA	1:C:283:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ASP:C	1:A:359:ASP:OD1	2.41	0.58
1:E:356:THR:O	1:E:358:ASP:OD1	2.22	0.58
1:C:328:THR:HG21	1:C:415:TYR:OH	2.03	0.58
1:A:228:LEU:HB2	1:A:289:TYR:HB3	1.85	0.58
1:B:163:GLN:O	1:B:167:ILE:HD13	2.03	0.58
1:B:167:ILE:O	1:B:168:ASN:HB3	2.03	0.58
1:E:43:ASN:HD21	1:E:113:LEU:H	1.51	0.58
1:B:328:THR:HG21	1:B:415:TYR:OH	2.04	0.58
1:B:59:LEU:C	1:B:61:SER:H	2.05	0.58
1:D:149:MET:C	1:D:151:GLU:H	2.06	0.58
1:C:9:ILE:HG23	1:C:10:ASP:N	2.18	0.58
1:E:364:LEU:O	1:E:366:THR:N	2.36	0.58
1:C:200:MET:HB2	1:C:277:TYR:CE2	2.39	0.58
1:B:172:GLU:CG	1:B:173:PRO:HD3	2.31	0.57
1:A:45:THR:O	1:A:45:THR:CG2	2.52	0.57
1:A:163:GLN:N	1:A:163:GLN:OE1	2.37	0.57
1:E:328:THR:CG2	1:E:415:TYR:HE1	2.17	0.57
1:B:228:LEU:HB2	1:B:289:TYR:HB3	1.86	0.57
1:A:59:LEU:C	1:A:61:SER:H	2.08	0.57
1:A:290:SER:HA	2:R:31:A:OP1	2.04	0.57
1:C:54:TYR:HD1	1:C:122:SER:HB2	1.69	0.57
1:A:175:VAL:HG13	1:A:181:ILE:HG12	1.86	0.57
1:E:317:ARG:HE	2:R:40:A:H3'	1.68	0.57
1:B:160:LEU:O	1:B:160:LEU:HD12	2.04	0.57
1:A:29:ALA:O	1:A:31:TYR:N	2.37	0.57
1:B:44:THR:HA	1:B:46:LYS:HD2	1.86	0.57
1:A:98:ALA:O	1:A:100:ASP:N	2.38	0.57
1:D:317:ARG:N	1:D:317:ARG:NH1	2.52	0.57
1:E:169:GLU:O	1:E:170:GLN:O	2.22	0.57
1:D:199:ASP:OD1	1:D:217:THR:HG23	2.03	0.57
1:A:354:LYS:HD3	1:E:379:LEU:HB3	1.86	0.57
1:E:401:VAL:O	1:E:404:LEU:HB2	2.05	0.57
1:E:44:THR:HG22	1:E:46:LYS:HZ3	1.68	0.57
1:E:328:THR:HG21	1:E:415:TYR:CE1	2.40	0.57
1:E:59:LEU:C	1:E:61:SER:H	2.08	0.57
1:A:127:THR:HG23	1:A:129:ALA:H	1.68	0.57
1:E:133:TRP:NE1	1:E:167:ILE:HG21	2.18	0.57
1:B:278:LEU:HA	1:B:283:LEU:HD12	1.85	0.57
1:A:167:ILE:O	1:A:169:GLU:OE2	2.22	0.57
1:B:137:TYR:CE2	1:B:141:LEU:HD11	2.39	0.57
1:C:317:ARG:HG3	1:C:410:LYS:NZ	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:THR:HG23	1:E:129:ALA:H	1.70	0.57
1:A:337:ALA:HA	1:A:378:TRP:CZ2	2.40	0.57
1:C:290:SER:HB2	2:R:12:A:H5'	1.86	0.57
1:D:127:THR:HG23	1:D:129:ALA:H	1.70	0.56
1:D:28:PRO:HD2	1:D:266:GLN:NE2	2.19	0.56
1:D:122:SER:O	1:D:123:ASP:HB2	2.04	0.56
1:C:44:THR:HG21	1:C:116:VAL:HG11	1.87	0.56
1:B:102:ILE:HB	1:B:106:ASP:OD2	2.05	0.56
1:C:25:VAL:HG11	1:C:288:PRO:HA	1.87	0.56
1:D:317:ARG:NH1	1:D:317:ARG:O	2.38	0.56
1:C:137:TYR:CE2	1:C:141:LEU:HD11	2.40	0.56
1:E:150:PRO:HA	1:E:152:TYR:HE1	1.66	0.56
1:B:298:HIS:NE2	1:B:317:ARG:NH2	2.54	0.56
1:A:328:THR:HG21	1:A:415:TYR:CE1	2.40	0.56
1:E:144:VAL:O	1:E:147:THR:HG22	2.05	0.56
1:B:67:ILE:HD12	1:B:67:ILE:H	1.68	0.56
1:C:127:THR:HG23	1:C:129:ALA:H	1.69	0.56
1:D:302:GLN:HG2	1:D:316:ALA:HB2	1.86	0.56
1:A:170:GLN:N	1:A:170:GLN:CD	2.58	0.56
1:A:164:CYS:HA	1:A:168:ASN:HA	1.88	0.56
1:D:317:ARG:NE	2:R:4:A:C2'	2.34	0.56
1:A:385:GLN:HG2	1:A:390:THR:CG2	2.36	0.56
1:D:59:LEU:C	1:D:61:SER:H	2.08	0.56
1:C:44:THR:HA	1:C:46:LYS:HZ2	1.69	0.56
1:D:163:GLN:OE1	1:D:163:GLN:N	2.34	0.56
1:A:344:LEU:HD13	1:E:250:LEU:HB3	1.87	0.56
1:D:328:THR:CG2	1:D:415:TYR:HE1	2.17	0.56
1:B:13:VAL:HG12	1:B:14:ILE:N	2.21	0.56
1:A:312:ARG:HG3	2:R:32:A:C4	2.41	0.56
1:C:226:ALA:HB2	2:R:13:A:C5'	2.33	0.56
1:A:294:ASN:N	1:A:295:PRO:HD3	2.21	0.56
1:C:42:ILE:HD12	1:C:74:TYR:CD2	2.40	0.56
1:C:385:GLN:HG2	1:C:390:THR:CG2	2.36	0.56
1:D:13:VAL:HG12	1:D:14:ILE:N	2.20	0.56
1:E:143:ARG:HH22	2:R:44:A:H3'	1.71	0.56
1:C:144:VAL:O	1:C:147:THR:HG22	2.06	0.56
1:E:13:VAL:HG12	1:E:14:ILE:N	2.21	0.56
1:A:317:ARG:HE	2:R:31:A:H2'	1.72	0.56
1:C:328:THR:HG21	1:C:415:TYR:CE1	2.40	0.56
1:D:144:VAL:O	1:D:147:THR:HG22	2.06	0.56
1:B:175:VAL:HG13	1:B:181:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:THR:HG21	1:B:415:TYR:CE1	2.40	0.55
1:B:41:TYR:CE1	1:B:110:LEU:HD12	2.41	0.55
1:B:253:GLU:N	1:B:253:GLU:CD	2.55	0.55
1:A:131:ASP:HA	1:A:135:PRO:HG2	1.88	0.55
1:A:278:LEU:HA	1:A:283:LEU:HD12	1.88	0.55
1:E:163:GLN:OE1	1:E:163:GLN:N	2.38	0.55
2:R:21:A:C6	2:R:22:A:N1	2.75	0.55
1:D:79:ASP:C	1:D:81:ARG:N	2.59	0.55
1:A:84:LEU:HD21	1:A:88:TRP:CE3	2.42	0.55
1:C:44:THR:HA	1:C:46:LYS:NZ	2.22	0.55
1:C:408:ARG:HD3	2:R:15:A:C6	2.41	0.55
1:E:44:THR:HA	1:E:46:LYS:HD2	1.87	0.55
1:B:149:MET:HG3	2:R:24:A:H1'	1.89	0.55
2:R:1:A:H2'	2:R:2:A:H5'	1.89	0.55
1:C:104:ILE:HG12	1:C:201:PHE:CG	2.42	0.55
1:B:408:ARG:HD3	2:R:24:A:C5	2.42	0.55
1:C:317:ARG:HG3	1:C:410:LYS:HZ1	1.72	0.55
1:B:163:GLN:N	1:B:163:GLN:OE1	2.37	0.55
1:D:228:LEU:HB2	1:D:289:TYR:HB3	1.88	0.55
1:E:174:LEU:N	1:E:174:LEU:HD12	2.22	0.55
1:D:171:PHE:CD2	1:D:172:GLU:N	2.74	0.55
1:B:298:HIS:CD2	1:B:317:ARG:HH12	2.19	0.55
1:C:224:ASP:HA	2:R:13:A:OP1	2.07	0.55
1:E:79:ASP:C	1:E:81:ARG:N	2.60	0.55
1:C:383:GLU:HG3	1:D:354:LYS:HE2	1.89	0.55
1:E:228:LEU:HB2	1:E:289:TYR:HB3	1.87	0.55
1:A:13:VAL:HG12	1:A:14:ILE:N	2.22	0.55
1:C:150:PRO:HA	1:C:152:TYR:HE1	1.67	0.55
1:E:40:LEU:HD22	1:E:42:ILE:HG13	1.88	0.55
1:B:323:GLU:O	1:B:327:LEU:HD22	2.06	0.55
1:A:41:TYR:CE1	1:A:110:LEU:HD12	2.42	0.55
1:A:232:GLY:HA2	1:E:18:LEU:HD12	1.89	0.55
1:D:44:THR:HA	1:D:46:LYS:NZ	2.23	0.54
1:B:298:HIS:NE2	1:B:317:ARG:CZ	2.70	0.54
1:C:28:PRO:O	1:C:31:TYR:HB3	2.07	0.54
1:C:354:LYS:HE3	1:C:356:THR:HB	1.88	0.54
1:B:127:THR:HG23	1:B:129:ALA:H	1.71	0.54
1:B:99:GLY:O	1:B:100:ASP:C	2.45	0.54
1:E:153:ARG:CZ	1:E:176:PRO:O	2.56	0.54
1:C:293:LYS:C	1:C:295:PRO:HD3	2.26	0.54
1:D:66:ILE:HD12	1:D:69:VAL:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ILE:CD1	1:A:74:TYR:HB2	2.37	0.54
1:B:354:LYS:HE3	1:B:356:THR:HB	1.88	0.54
1:E:238:THR:HG22	1:E:308:LEU:HD23	1.89	0.54
1:C:67:ILE:HD12	1:C:67:ILE:H	1.72	0.54
1:D:44:THR:HG22	1:D:46:LYS:HZ3	1.73	0.54
1:D:43:ASN:ND2	1:D:113:LEU:H	2.06	0.54
1:D:28:PRO:O	1:D:31:TYR:HB3	2.08	0.54
1:A:328:THR:HG21	1:A:415:TYR:OH	2.07	0.54
1:E:131:ASP:HA	1:E:135:PRO:HG2	1.88	0.54
1:B:2:SER:O	1:C:243:GLU:HG3	2.07	0.54
1:D:102:ILE:HB	1:D:106:ASP:OD2	2.06	0.54
1:E:336:TYR:CD1	1:E:393:MET:HB3	2.43	0.54
1:E:228:LEU:HD11	1:E:268:ILE:HG22	1.89	0.54
1:C:401:VAL:O	1:C:404:LEU:HB2	2.07	0.54
1:D:30:ASP:CG	1:D:33:ARG:HH21	2.11	0.54
2:R:19:A:H2'	2:R:20:A:O4'	2.07	0.54
1:B:312:ARG:HG3	2:R:23:A:C4	2.43	0.54
1:B:293:LYS:C	1:B:295:PRO:HD3	2.28	0.54
1:E:257:GLU:OE1	1:E:295:PRO:HD2	2.08	0.54
1:E:385:GLN:HG2	1:E:390:THR:CG2	2.38	0.54
1:D:150:PRO:HA	1:D:152:TYR:HE1	1.69	0.54
1:D:149:MET:HG3	2:R:6:A:N9	2.22	0.54
1:D:44:THR:HA	1:D:46:LYS:HD2	1.87	0.54
1:B:149:MET:HG3	2:R:24:A:C1'	2.38	0.54
1:C:149:MET:O	1:C:152:TYR:CG	2.61	0.54
1:A:354:LYS:HE2	1:E:383:GLU:HG3	1.89	0.54
1:E:29:ALA:O	1:E:31:TYR:N	2.39	0.54
1:D:385:GLN:HG2	1:D:390:THR:CG2	2.38	0.54
1:B:172:GLU:CB	1:B:173:PRO:CD	2.28	0.54
1:B:257:GLU:OE1	1:B:295:PRO:HD2	2.07	0.54
1:A:253:GLU:N	1:A:253:GLU:CD	2.57	0.54
1:B:131:ASP:HA	1:B:135:PRO:HG2	1.90	0.54
1:D:293:LYS:C	1:D:295:PRO:HD3	2.28	0.54
1:D:42:ILE:CD1	1:D:74:TYR:HB2	2.38	0.54
1:D:131:ASP:HA	1:D:135:PRO:HG2	1.89	0.54
1:A:104:ILE:HG12	1:A:201:PHE:CG	2.42	0.54
1:D:215:TYR:CD2	1:D:215:TYR:C	2.81	0.54
1:C:215:TYR:CD2	1:C:215:TYR:C	2.80	0.54
1:D:149:MET:HG3	2:R:6:A:C1'	2.37	0.54
1:C:199:ASP:OD1	1:C:217:THR:HG23	2.08	0.54
1:D:98:ALA:C	1:D:100:ASP:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LYS:O	1:C:167:ILE:HG23	2.08	0.54
1:D:354:LYS:HE3	1:D:356:THR:HB	1.89	0.54
1:B:390:THR:O	1:B:393:MET:HG2	2.07	0.54
1:D:182:PHE:C	1:D:184:VAL:H	2.10	0.54
1:D:41:TYR:CE1	1:D:110:LEU:HD12	2.42	0.54
1:C:184:VAL:HG22	1:D:165:LYS:HG3	1.89	0.54
1:E:150:PRO:N	1:E:152:TYR:CE1	2.76	0.54
1:B:182:PHE:C	1:B:184:VAL:H	2.11	0.54
1:E:15:VAL:HB	1:E:17:LYS:NZ	2.23	0.54
1:A:398:LYS:O	1:A:402:MET:HG2	2.08	0.54
1:A:279:ILE:HD11	1:A:287:SER:HB3	1.88	0.53
1:E:290:SER:HB2	2:R:39:A:H5'	1.88	0.53
1:D:257:GLU:OE1	1:D:295:PRO:HD2	2.07	0.53
1:E:41:TYR:CE1	1:E:110:LEU:HD12	2.43	0.53
1:A:182:PHE:C	1:A:184:VAL:H	2.11	0.53
1:A:336:TYR:CD1	1:A:393:MET:HB3	2.42	0.53
1:D:312:ARG:HG3	2:R:5:A:C4	2.42	0.53
1:E:354:LYS:HE3	1:E:356:THR:HB	1.89	0.53
2:R:25:A:H2'	2:R:26:A:C8	2.42	0.53
1:E:149:MET:C	1:E:151:GLU:N	2.62	0.53
1:B:376:VAL:HG22	1:C:346:GLN:OE1	2.09	0.53
1:C:66:ILE:HD12	1:C:69:VAL:CG2	2.38	0.53
1:D:303:LEU:CD2	1:D:328:THR:HA	2.38	0.53
1:D:44:THR:HA	1:D:46:LYS:HZ2	1.74	0.53
1:C:43:ASN:HD21	1:C:113:LEU:H	1.55	0.53
1:C:317:ARG:O	1:C:319:PRO:HD3	2.08	0.53
1:E:109:SER:O	1:E:110:LEU:HD23	2.09	0.53
1:E:182:PHE:C	1:E:184:VAL:H	2.10	0.53
2:R:10:A:C5'	2:R:10:A:C8	2.86	0.53
1:A:150:PRO:HA	1:A:152:TYR:HE1	1.70	0.53
1:E:28:PRO:O	1:E:31:TYR:HB3	2.08	0.53
1:D:407:LEU:HD13	1:D:413:GLY:C	2.29	0.53
1:D:165:LYS:HB3	1:D:166:MET:HE3	1.90	0.53
1:A:365:THR:HG23	1:A:366:THR:HG22	1.89	0.53
1:E:177:GLU:HA	1:E:181:ILE:CD1	2.32	0.53
1:C:278:LEU:HD23	1:C:279:ILE:H	1.73	0.53
1:C:180:ASP:C	1:C:180:ASP:OD2	2.46	0.53
1:A:379:LEU:CD1	1:B:346:GLN:HB2	2.39	0.53
1:D:337:ALA:HA	1:D:378:TRP:CZ2	2.44	0.53
1:E:104:ILE:HG12	1:E:201:PHE:CG	2.44	0.53
1:B:365:THR:HG22	1:B:368:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:MET:HG3	2:R:6:A:H1'	1.90	0.53
1:B:184:VAL:CG1	1:C:166:MET:H	2.15	0.53
1:B:167:ILE:HG22	1:B:168:ASN:N	2.23	0.53
1:E:105:PHE:C	1:E:107:LEU:N	2.62	0.53
1:A:238:THR:C	1:A:240:MET:N	2.61	0.53
1:A:215:TYR:C	1:A:215:TYR:CD2	2.81	0.53
2:R:29:A:H2'	2:R:30:A:H5"	1.91	0.53
1:A:317:ARG:NH2	2:R:32:A:OP1	2.41	0.53
1:E:302:GLN:HG3	1:E:313:ALA:CB	2.38	0.53
1:B:158:ASP:C	1:B:160:LEU:N	2.62	0.53
1:D:278:LEU:HD23	1:D:279:ILE:H	1.72	0.53
2:R:1:A:H8	2:R:1:A:O5'	1.92	0.53
1:E:18:LEU:HB2	1:E:19:PRO:HD2	1.91	0.53
1:D:292:VAL:HG13	2:R:3:A:H5"	1.91	0.53
1:D:42:ILE:HD12	1:D:74:TYR:CD2	2.43	0.53
1:D:401:VAL:O	1:D:404:LEU:HB2	2.09	0.53
1:A:160:LEU:HD12	1:A:160:LEU:O	2.08	0.53
1:A:402:MET:SD	1:E:422:LYS:HD2	2.49	0.53
1:B:44:THR:HA	1:B:46:LYS:HE3	1.90	0.53
1:C:317:ARG:NE	2:R:13:A:O2'	2.42	0.53
1:E:294:ASN:N	1:E:295:PRO:HD3	2.23	0.53
1:A:184:VAL:HG12	1:B:166:MET:HE2	1.91	0.53
1:A:18:LEU:CD1	1:B:232:GLY:HA2	2.39	0.53
1:C:228:LEU:HB2	1:C:289:TYR:HB3	1.91	0.53
1:A:401:VAL:O	1:A:404:LEU:HB2	2.09	0.53
1:E:261:MET:HB3	1:E:262:MET:HE3	1.91	0.53
1:A:352:ASP:OD1	1:E:376:VAL:HG21	2.09	0.52
1:D:149:MET:C	1:D:151:GLU:N	2.62	0.52
1:D:177:GLU:CA	1:D:181:ILE:HD11	2.32	0.52
2:R:39:A:H5'	2:R:40:A:OP2	2.10	0.52
1:B:317:ARG:NH2	1:B:317:ARG:H	2.07	0.52
1:C:317:ARG:CZ	1:C:317:ARG:N	2.71	0.52
1:A:40:LEU:HD22	1:A:42:ILE:HG13	1.91	0.52
1:C:79:ASP:C	1:C:81:ARG:N	2.61	0.52
1:A:376:VAL:HG22	1:B:346:GLN:OE1	2.10	0.52
1:C:15:VAL:HB	1:C:17:LYS:NZ	2.23	0.52
1:E:243:GLU:O	1:E:247:THR:HG23	2.09	0.52
1:C:308:LEU:O	1:C:309:ARG:HB2	2.10	0.52
1:A:7:ARG:O	1:A:11:ASN:HA	2.10	0.52
1:E:412:ILE:C	1:E:412:ILE:HD12	2.29	0.52
1:B:180:ASP:OD2	1:B:180:ASP:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:PRO:O	1:A:31:TYR:HB3	2.09	0.52
1:E:37:GLU:O	1:E:39:PRO:HD3	2.09	0.52
1:D:328:THR:HG21	1:D:415:TYR:CE1	2.44	0.52
1:C:84:LEU:HD21	1:C:88:TRP:CE3	2.43	0.52
2:R:6:A:C5'	2:R:7:A:O5'	2.54	0.52
1:A:153:ARG:CZ	1:A:176:PRO:O	2.58	0.52
1:B:44:THR:HG22	1:B:46:LYS:NZ	2.24	0.52
1:C:150:PRO:N	1:C:152:TYR:CE1	2.77	0.52
1:E:298:HIS:NE2	1:E:317:ARG:NH1	2.57	0.52
1:E:43:ASN:ND2	1:E:113:LEU:H	2.07	0.52
1:C:165:LYS:N	1:C:167:ILE:HG12	2.24	0.52
1:B:238:THR:HG22	1:B:308:LEU:HD23	1.91	0.52
1:C:328:THR:CG2	1:C:415:TYR:CE1	2.93	0.52
1:D:291:SER:HB3	2:R:4:A:OP2	2.09	0.52
1:E:317:ARG:H	1:E:317:ARG:NH2	2.06	0.52
1:A:42:ILE:HD12	1:A:74:TYR:CD2	2.45	0.52
1:E:303:LEU:CD2	1:E:328:THR:HA	2.40	0.52
1:A:184:VAL:HG12	1:B:166:MET:CE	2.40	0.52
1:D:390:THR:O	1:D:393:MET:HG2	2.09	0.52
1:B:401:VAL:O	1:B:404:LEU:HB2	2.09	0.52
1:E:84:LEU:HD21	1:E:88:TRP:CE3	2.45	0.52
1:B:199:ASP:OD1	1:B:217:THR:HG23	2.09	0.52
1:B:153:ARG:CZ	1:B:176:PRO:O	2.58	0.52
1:B:105:PHE:C	1:B:107:LEU:N	2.61	0.52
1:D:67:ILE:HD12	1:D:67:ILE:H	1.74	0.52
1:D:149:MET:O	1:D:152:TYR:CD1	2.63	0.52
1:B:149:MET:C	1:B:151:GLU:N	2.61	0.52
1:C:181:ILE:CD1	1:C:181:ILE:H	2.11	0.52
1:A:354:LYS:HE3	1:A:356:THR:HB	1.91	0.52
1:E:295:PRO:HB2	1:E:322:ILE:CG2	2.40	0.52
1:B:336:TYR:CD1	1:B:393:MET:HB3	2.44	0.52
1:B:332:LEU:HD13	1:B:393:MET:HE2	1.90	0.52
1:B:104:ILE:HG12	1:B:201:PHE:CG	2.44	0.52
1:D:148:GLN:NE2	1:D:179:ARG:NE	2.56	0.52
1:E:177:GLU:CA	1:E:181:ILE:HD11	2.32	0.52
1:C:27:TYR:HB3	1:C:266:GLN:HE22	1.74	0.52
1:C:37:GLU:O	1:C:39:PRO:HD3	2.10	0.52
1:B:379:LEU:CD1	1:C:346:GLN:HB2	2.40	0.52
1:A:358:ASP:O	1:A:359:ASP:C	2.48	0.52
1:B:15:VAL:HB	1:B:17:LYS:NZ	2.24	0.52
1:E:149:MET:HG3	2:R:42:A:N9	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:MET:O	1:E:152:TYR:CG	2.63	0.52
1:A:133:TRP:CD1	1:A:167:ILE:CG2	2.89	0.52
1:C:298:HIS:NE2	1:C:317:ARG:NH2	2.58	0.52
1:B:160:LEU:C	1:B:160:LEU:HD12	2.31	0.52
1:C:160:LEU:O	1:C:160:LEU:HD12	2.10	0.52
1:E:42:ILE:HD12	1:E:74:TYR:CD2	2.45	0.52
1:A:15:VAL:HB	1:A:17:LYS:NZ	2.25	0.52
1:D:412:ILE:C	1:D:412:ILE:HD12	2.29	0.52
1:B:172:GLU:HB3	1:B:173:PRO:HD3	0.59	0.51
1:D:270:LYS:HB3	1:D:273:SER:HB2	1.92	0.51
1:D:177:GLU:HA	1:D:181:ILE:CD1	2.32	0.51
1:E:356:THR:HG23	1:E:357:PRO:CD	2.25	0.51
1:B:149:MET:O	1:B:152:TYR:CG	2.63	0.51
1:B:295:PRO:HB2	1:B:322:ILE:CG2	2.40	0.51
1:C:165:LYS:O	1:C:167:ILE:N	2.42	0.51
1:B:215:TYR:C	1:B:215:TYR:CD2	2.84	0.51
1:A:164:CYS:HB3	1:E:180:ASP:OD2	2.10	0.51
1:D:313:ALA:O	1:D:314:ARG:C	2.48	0.51
1:D:44:THR:HG22	1:D:46:LYS:NZ	2.25	0.51
1:A:199:ASP:OD1	1:A:214:ARG:HD2	2.10	0.51
1:B:44:THR:HA	1:B:46:LYS:NZ	2.25	0.51
1:B:84:LEU:HD21	1:B:88:TRP:CE3	2.45	0.51
1:D:160:LEU:HD12	1:D:160:LEU:C	2.31	0.51
1:C:180:ASP:OD2	1:D:164:CYS:HB3	2.10	0.51
1:E:122:SER:O	1:E:123:ASP:HB2	2.10	0.51
1:B:7:ARG:O	1:B:11:ASN:HA	2.10	0.51
1:D:314:ARG:NH1	1:D:405:GLN:O	2.43	0.51
1:A:356:THR:CG2	1:A:357:PRO:HD3	2.32	0.51
1:A:293:LYS:C	1:A:295:PRO:HD3	2.30	0.51
1:A:18:LEU:HD12	1:B:232:GLY:CA	2.40	0.51
1:E:401:VAL:HG21	1:E:420:PHE:HB2	1.92	0.51
1:A:199:ASP:OD1	1:A:217:THR:HG23	2.11	0.51
1:B:153:ARG:CZ	1:B:176:PRO:CA	2.88	0.51
1:E:313:ALA:O	1:E:314:ARG:C	2.49	0.51
1:E:317:ARG:NH1	1:E:317:ARG:N	2.59	0.51
1:B:168:ASN:O	1:B:169:GLU:HB3	2.10	0.51
1:D:238:THR:HG22	1:D:308:LEU:HD23	1.92	0.51
1:A:228:LEU:HD11	1:A:268:ILE:HG22	1.93	0.51
1:E:235:CYS:HA	1:E:245:VAL:HG21	1.92	0.51
1:C:412:ILE:HD12	1:C:412:ILE:C	2.30	0.51
1:C:149:MET:C	1:C:151:GLU:N	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ALA:HA	1:B:378:TRP:CZ2	2.46	0.51
1:D:153:ARG:CZ	1:D:176:PRO:CA	2.87	0.51
1:D:84:LEU:HD21	1:D:88:TRP:CE3	2.45	0.51
1:C:133:TRP:O	1:C:136:LEU:N	2.44	0.51
1:C:7:ARG:O	1:C:11:ASN:HA	2.10	0.51
1:B:177:GLU:CA	1:B:181:ILE:HD11	2.32	0.51
2:R:27:A:H2'	2:R:28:A:O4'	2.11	0.51
1:A:169:GLU:HA	1:A:170:GLN:NE2	2.25	0.51
1:B:328:THR:CG2	1:B:415:TYR:CE1	2.94	0.51
1:C:131:ASP:HA	1:C:135:PRO:HG2	1.93	0.51
1:A:314:ARG:NH1	1:A:405:GLN:O	2.44	0.51
2:R:3:A:C6	2:R:4:A:C6	2.99	0.51
1:B:43:ASN:OD1	1:B:112:ALA:CB	2.54	0.51
1:E:160:LEU:HD12	1:E:160:LEU:O	2.11	0.51
1:D:117:LEU:CB	1:D:118:PRO:CD	2.87	0.51
1:E:365:THR:O	1:E:365:THR:HG23	2.11	0.51
1:A:79:ASP:C	1:A:81:ARG:N	2.60	0.51
1:E:40:LEU:HD11	1:E:194:ILE:HG12	1.91	0.51
1:B:278:LEU:HD23	1:B:279:ILE:H	1.76	0.51
1:A:66:ILE:HD12	1:A:69:VAL:CG2	2.39	0.50
1:C:174:LEU:N	1:C:174:LEU:HD12	2.26	0.50
1:E:30:ASP:CG	1:E:33:ARG:HH21	2.14	0.50
1:C:314:ARG:NH1	1:C:405:GLN:O	2.44	0.50
1:D:31:TYR:C	1:D:31:TYR:CD1	2.84	0.50
1:E:337:ALA:HA	1:E:378:TRP:CZ2	2.46	0.50
1:A:234:LEU:HD11	1:A:304:THR:HG21	1.93	0.50
1:B:42:ILE:HD12	1:B:74:TYR:HD2	1.75	0.50
1:A:149:MET:C	1:A:151:GLU:N	2.61	0.50
1:A:149:MET:O	1:A:152:TYR:CG	2.65	0.50
1:A:302:GLN:HG3	1:A:313:ALA:CB	2.41	0.50
1:B:148:GLN:NE2	1:B:179:ARG:NE	2.57	0.50
1:E:153:ARG:CZ	1:E:176:PRO:CA	2.87	0.50
1:C:42:ILE:CD1	1:C:74:TYR:HB2	2.39	0.50
1:D:332:LEU:HD13	1:D:393:MET:HE2	1.92	0.50
1:A:87:ASP:OD2	1:A:97:LYS:HA	2.11	0.50
1:C:41:TYR:CE1	1:C:110:LEU:HD12	2.46	0.50
1:D:104:ILE:O	1:D:104:ILE:HG22	2.10	0.50
1:D:150:PRO:N	1:D:152:TYR:CE1	2.80	0.50
1:B:44:THR:HA	1:B:46:LYS:HZ2	1.75	0.50
1:E:44:THR:HG22	1:E:46:LYS:NZ	2.25	0.50
1:A:165:LYS:O	1:A:167:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:SER:N	2:R:13:A:OP2	2.44	0.50
1:E:180:ASP:OD2	1:E:180:ASP:C	2.45	0.50
1:E:43:ASN:HA	1:E:111:LYS:HG3	1.93	0.50
1:D:336:TYR:CD1	1:D:393:MET:HB3	2.47	0.50
1:A:47:SER:HB3	1:A:50:ASP:HB2	1.93	0.50
1:C:182:PHE:C	1:C:184:VAL:H	2.14	0.50
1:C:298:HIS:HD2	1:C:317:ARG:NH1	2.10	0.50
1:A:295:PRO:HB2	1:A:322:ILE:CG2	2.41	0.50
1:C:286:LYS:HD2	2:R:12:A:OP2	2.10	0.50
1:A:40:LEU:HD11	1:A:194:ILE:HG12	1.92	0.50
1:C:122:SER:O	1:C:123:ASP:HB2	2.11	0.50
1:B:104:ILE:O	1:B:104:ILE:HG22	2.11	0.50
1:A:412:ILE:HD12	1:A:412:ILE:C	2.32	0.50
1:D:292:VAL:HG11	2:R:3:A:H5"	1.94	0.50
2:R:29:A:C3'	2:R:30:A:H5"	2.42	0.50
1:B:46:LYS:O	1:B:47:SER:C	2.49	0.50
1:D:43:ASN:HA	1:D:111:LYS:HG3	1.94	0.50
1:A:308:LEU:O	1:A:309:ARG:HB2	2.12	0.50
1:C:390:THR:O	1:C:393:MET:HG2	2.12	0.50
2:R:1:A:H2'	2:R:2:A:C5'	2.41	0.50
1:D:398:LYS:O	1:D:402:MET:HG2	2.12	0.50
1:C:178:GLY:O	1:C:179:ARG:C	2.51	0.50
1:A:165:LYS:C	1:A:167:ILE:N	2.65	0.50
1:A:180:ASP:OD2	1:A:180:ASP:C	2.48	0.50
1:B:28:PRO:O	1:B:31:TYR:HB3	2.12	0.50
1:A:97:LYS:O	1:A:98:ALA:C	2.50	0.50
1:A:303:LEU:CD2	1:A:328:THR:HA	2.42	0.50
1:B:109:SER:O	1:B:110:LEU:HD23	2.12	0.50
1:C:148:GLN:NE2	1:C:179:ARG:NE	2.57	0.50
1:C:356:THR:N	1:C:357:PRO:CD	2.75	0.50
1:E:66:ILE:HD12	1:E:69:VAL:CG2	2.40	0.50
1:A:184:VAL:HG11	1:B:166:MET:HG2	1.94	0.50
1:B:412:ILE:HD12	1:B:412:ILE:C	2.32	0.50
2:R:34:A:OP2	2:R:34:A:H4'	2.11	0.49
1:C:44:THR:HG22	1:C:46:LYS:HZ3	1.77	0.49
1:D:128:SER:CA	1:D:130:ASP:HB2	2.40	0.49
1:C:153:ARG:CZ	1:C:176:PRO:CA	2.90	0.49
1:E:408:ARG:HD3	2:R:42:A:C5	2.47	0.49
1:A:238:THR:HG22	1:A:308:LEU:HD23	1.94	0.49
1:E:46:LYS:O	1:E:47:SER:C	2.50	0.49
1:A:363:GLY:O	1:A:365:THR:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:GLU:N	1:C:253:GLU:CD	2.61	0.49
1:D:43:ASN:ND2	1:D:113:LEU:N	2.59	0.49
1:D:365:THR:HG23	1:D:366:THR:N	2.27	0.49
1:D:317:ARG:NH2	2:R:4:A:O3'	2.44	0.49
1:C:44:THR:HG22	1:C:46:LYS:NZ	2.26	0.49
1:D:149:MET:CG	2:R:6:A:H1'	2.42	0.49
1:C:199:ASP:OD1	1:C:214:ARG:HD2	2.12	0.49
1:B:302:GLN:HG3	1:B:313:ALA:CB	2.42	0.49
1:A:38:ILE:O	1:A:38:ILE:HD12	2.12	0.49
1:E:293:LYS:C	1:E:295:PRO:HD3	2.32	0.49
1:E:43:ASN:ND2	1:E:113:LEU:N	2.59	0.49
1:A:380:GLY:N	1:B:354:LYS:HD2	2.28	0.49
1:D:15:VAL:HB	1:D:17:LYS:NZ	2.27	0.49
1:D:148:GLN:CD	1:D:179:ARG:HE	2.15	0.49
1:A:181:ILE:H	1:A:181:ILE:CD1	2.06	0.49
1:A:408:ARG:HD3	2:R:33:A:C6	2.46	0.49
1:B:178:GLY:O	1:B:179:ARG:C	2.50	0.49
1:D:295:PRO:HB2	1:D:322:ILE:CG2	2.43	0.49
1:A:309:ARG:HG2	1:E:415:TYR:HE2	1.77	0.49
1:A:18:LEU:HB2	1:A:19:PRO:HD2	1.93	0.49
1:C:109:SER:O	1:C:110:LEU:HD23	2.12	0.49
1:B:234:LEU:HD11	1:B:304:THR:HG21	1.95	0.49
1:E:398:LYS:O	1:E:402:MET:HG2	2.12	0.49
1:D:298:HIS:NE2	1:D:317:ARG:NH1	2.60	0.49
1:D:166:MET:C	1:D:167:ILE:HG13	2.27	0.49
1:D:87:ASP:OD2	1:D:97:LYS:HA	2.13	0.49
1:C:153:ARG:CZ	1:C:176:PRO:O	2.61	0.49
1:E:317:ARG:NH1	1:E:317:ARG:O	2.45	0.49
1:B:299:PHE:HZ	1:B:415:TYR:CE1	2.31	0.49
1:C:104:ILE:HG22	1:C:104:ILE:O	2.11	0.49
1:E:104:ILE:HG22	1:E:104:ILE:O	2.12	0.49
1:A:247:THR:HA	1:B:348:PHE:HB2	1.95	0.49
1:A:257:GLU:OE1	1:A:295:PRO:HD2	2.12	0.49
1:D:356:THR:N	1:D:357:PRO:CD	2.75	0.49
1:D:317:ARG:H	1:D:317:ARG:NH2	2.09	0.49
1:E:166:MET:O	1:E:167:ILE:HG13	2.12	0.49
1:B:314:ARG:NH1	1:B:405:GLN:O	2.44	0.49
1:C:18:LEU:HB2	1:C:19:PRO:HD2	1.95	0.49
1:D:253:GLU:N	1:D:253:GLU:CD	2.61	0.49
1:E:38:ILE:HD11	1:E:107:LEU:HB3	1.95	0.49
1:C:295:PRO:HB2	1:C:322:ILE:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:THR:N	1:B:357:PRO:CD	2.76	0.49
1:B:303:LEU:CD2	1:B:328:THR:HA	2.43	0.49
1:B:2:SER:HA	1:D:350:VAL:HG21	1.94	0.49
1:B:152:TYR:HD1	1:B:153:ARG:N	2.09	0.49
1:A:160:LEU:C	1:A:160:LEU:HD12	2.32	0.49
1:E:314:ARG:NH1	1:E:405:GLN:O	2.45	0.49
1:B:163:GLN:O	1:B:167:ILE:CD1	2.61	0.49
1:B:38:ILE:O	1:B:38:ILE:HD12	2.13	0.49
1:D:40:LEU:HD22	1:D:42:ILE:HG13	1.95	0.49
1:E:279:ILE:HD11	1:E:287:SER:HB3	1.95	0.49
1:C:380:GLY:N	1:D:354:LYS:HD2	2.28	0.49
1:D:235:CYS:HA	1:D:245:VAL:HG21	1.95	0.49
1:D:401:VAL:HG21	1:D:420:PHE:HB2	1.95	0.49
1:C:170:GLN:CG	1:C:171:PHE:H	2.26	0.49
1:D:291:SER:N	2:R:4:A:OP2	2.45	0.49
1:A:153:ARG:CZ	1:A:176:PRO:CA	2.90	0.49
1:C:46:LYS:O	1:C:47:SER:C	2.51	0.49
1:E:158:ASP:C	1:E:160:LEU:N	2.66	0.49
1:C:172:GLU:CB	1:C:173:PRO:CD	2.90	0.49
1:B:143:ARG:HE	1:B:155:LYS:HE2	1.78	0.49
1:C:42:ILE:HD12	1:C:74:TYR:HD2	1.78	0.49
1:B:398:LYS:O	1:B:402:MET:HG2	2.12	0.49
1:D:91:PHE:CZ	1:D:267:GLU:HG3	2.48	0.49
1:E:215:TYR:C	1:E:215:TYR:CD2	2.85	0.49
1:E:307:LEU:HB3	1:E:335:ALA:HB1	1.95	0.49
1:D:152:TYR:HD1	1:D:153:ARG:N	2.08	0.48
1:B:150:PRO:HA	1:B:152:TYR:HE1	1.71	0.48
1:E:153:ARG:NH2	1:E:176:PRO:O	2.46	0.48
1:E:29:ALA:HB3	1:E:266:GLN:OE1	2.12	0.48
1:B:79:ASP:C	1:B:81:ARG:N	2.61	0.48
1:D:328:THR:CG2	1:D:415:TYR:CE1	2.96	0.48
1:D:104:ILE:HG12	1:D:201:PHE:CG	2.48	0.48
2:R:21:A:C6	2:R:22:A:C6	3.01	0.48
1:A:383:GLU:HG2	1:A:387:ARG:HD3	1.95	0.48
1:A:109:SER:O	1:A:110:LEU:HD23	2.13	0.48
1:B:97:LYS:O	1:B:98:ALA:C	2.51	0.48
1:C:302:GLN:HG3	1:C:313:ALA:CB	2.43	0.48
1:C:38:ILE:O	1:C:38:ILE:HD12	2.13	0.48
1:B:238:THR:C	1:B:240:MET:N	2.66	0.48
1:E:7:ARG:O	1:E:11:ASN:HA	2.14	0.48
1:A:270:LYS:HB3	1:A:273:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ALA:HB2	2:R:31:A:H5'	1.90	0.48
1:E:199:ASP:OD1	1:E:214:ARG:HD2	2.11	0.48
1:B:87:ASP:OD2	1:B:97:LYS:HA	2.12	0.48
1:D:163:GLN:HA	1:D:166:MET:CG	2.37	0.48
1:E:150:PRO:HD3	1:E:152:TYR:OH	2.13	0.48
1:E:312:ARG:HG3	2:R:41:A:C4	2.49	0.48
1:A:105:PHE:C	1:A:107:LEU:N	2.66	0.48
1:E:279:ILE:HD11	1:E:287:SER:CB	2.44	0.48
1:D:263:LEU:HG	1:D:264:PRO:CD	2.43	0.48
1:E:336:TYR:O	1:E:337:ALA:C	2.52	0.48
1:A:150:PRO:N	1:A:152:TYR:CE1	2.82	0.48
1:D:97:LYS:O	1:D:98:ALA:C	2.51	0.48
2:R:26:A:H3'	2:R:26:A:C8	2.48	0.48
1:E:408:ARG:HD3	2:R:42:A:C6	2.48	0.48
1:A:356:THR:N	1:A:357:PRO:CD	2.75	0.48
1:E:9:ILE:CG2	1:E:10:ASP:H	2.21	0.48
1:C:165:LYS:C	1:C:167:ILE:H	2.16	0.48
1:E:328:THR:CG2	1:E:415:TYR:CE1	2.95	0.48
1:C:325:THR:CG2	1:D:309:ARG:HH11	2.27	0.48
1:B:174:LEU:H	1:B:174:LEU:HD23	1.78	0.48
1:A:278:LEU:HD23	1:A:279:ILE:H	1.78	0.48
2:R:16:A:OP2	2:R:16:A:H4'	2.13	0.48
1:A:158:ASP:C	1:A:160:LEU:N	2.67	0.48
1:C:106:ASP:C	1:C:107:LEU:HD12	2.33	0.48
1:E:223:LYS:O	1:E:224:ASP:HB2	2.14	0.48
1:D:320:ASP:HA	1:D:324:TYR:HH	1.79	0.48
1:D:200:MET:HB2	1:D:277:TYR:CE2	2.48	0.48
1:C:303:LEU:CD2	1:C:328:THR:HA	2.43	0.48
1:D:136:LEU:HD13	1:D:163:GLN:HG3	1.96	0.48
1:C:247:THR:HA	1:D:348:PHE:HB2	1.96	0.48
1:E:323:GLU:O	1:E:327:LEU:HD22	2.13	0.48
1:C:270:LYS:HB3	1:C:273:SER:HB2	1.96	0.48
1:C:30:ASP:CG	1:C:33:ARG:HH21	2.17	0.48
2:R:29:A:H3'	2:R:30:A:H5"	1.95	0.48
1:B:44:THR:CA	1:B:46:LYS:CD	2.91	0.48
1:B:199:ASP:HB2	1:B:217:THR:HG23	1.95	0.48
1:D:158:ASP:C	1:D:160:LEU:N	2.68	0.48
1:B:38:ILE:HD11	1:B:107:LEU:CB	2.44	0.48
1:C:238:THR:HG22	1:C:308:LEU:HD23	1.94	0.48
1:E:215:TYR:HA	2:R:45:A:H4'	1.95	0.48
1:A:30:ASP:CG	1:A:33:ARG:HH21	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:ARG:HH22	2:R:8:A:H3'	1.79	0.48
1:D:302:GLN:HG3	1:D:313:ALA:CB	2.43	0.48
1:B:42:ILE:O	1:B:111:LYS:HG3	2.14	0.48
1:C:223:LYS:O	1:C:224:ASP:HB2	2.14	0.48
1:B:66:ILE:HD12	1:B:69:VAL:CG2	2.43	0.48
1:C:337:ALA:HA	1:C:378:TRP:CZ2	2.49	0.48
2:R:26:A:H4'	2:R:27:A:OP1	2.13	0.47
1:C:149:MET:O	1:C:152:TYR:CD1	2.67	0.47
1:C:151:GLU:O	1:C:155:LYS:HB2	2.14	0.47
1:D:105:PHE:C	1:D:107:LEU:N	2.61	0.47
1:A:166:MET:N	1:E:184:VAL:HG11	2.29	0.47
1:C:299:PHE:HZ	1:C:415:TYR:CE1	2.32	0.47
1:C:234:LEU:HD11	1:C:304:THR:HG21	1.96	0.47
1:C:304:THR:HG22	1:C:305:ALA:N	2.29	0.47
1:D:148:GLN:C	1:D:152:TYR:CE2	2.88	0.47
1:D:46:LYS:O	1:D:47:SER:C	2.50	0.47
1:B:44:THR:HG22	1:B:46:LYS:HZ3	1.79	0.47
1:A:165:LYS:O	1:A:167:ILE:CG1	2.62	0.47
1:C:31:TYR:CD1	1:C:31:TYR:C	2.88	0.47
1:E:320:ASP:HA	1:E:324:TYR:HH	1.79	0.47
1:A:328:THR:HG21	1:A:415:TYR:HE1	1.77	0.47
1:E:234:LEU:HD11	1:E:304:THR:HG21	1.94	0.47
1:B:200:MET:HB2	1:B:277:TYR:CE2	2.49	0.47
1:A:323:GLU:O	1:A:327:LEU:HD22	2.14	0.47
1:A:230:THR:HG21	1:A:298:HIS:ND1	2.29	0.47
1:C:43:ASN:ND2	1:C:113:LEU:H	2.12	0.47
1:D:268:ILE:H	1:D:268:ILE:HG12	1.32	0.47
2:R:34:A:H2'	2:R:35:A:O4'	2.15	0.47
1:E:42:ILE:CD1	1:E:74:TYR:HB2	2.42	0.47
1:D:238:THR:C	1:D:240:MET:N	2.66	0.47
1:E:270:LYS:HB3	1:E:273:SER:HB2	1.96	0.47
1:E:38:ILE:HD11	1:E:107:LEU:CB	2.44	0.47
1:D:153:ARG:CZ	1:D:176:PRO:O	2.62	0.47
1:C:44:THR:HA	1:C:46:LYS:HD2	1.90	0.47
1:E:160:LEU:HD12	1:E:160:LEU:C	2.35	0.47
1:E:143:ARG:HE	1:E:155:LYS:HE2	1.80	0.47
1:C:43:ASN:HA	1:C:111:LYS:HG3	1.97	0.47
1:B:18:LEU:HB2	1:B:19:PRO:HD2	1.95	0.47
1:A:235:CYS:HA	1:A:245:VAL:HG21	1.95	0.47
1:E:374:ASP:OD1	1:E:376:VAL:N	2.47	0.47
1:C:177:GLU:HA	1:C:181:ILE:CD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ARG:HE	1:C:155:LYS:HE2	1.80	0.47
1:E:151:GLU:O	1:E:155:LYS:HB2	2.15	0.47
1:E:149:MET:O	1:E:152:TYR:CD1	2.68	0.47
1:A:136:LEU:HD13	1:A:163:GLN:HG3	1.96	0.47
1:C:117:LEU:CB	1:C:118:PRO:CD	2.87	0.47
1:E:250:LEU:HD22	1:E:379:LEU:HD21	1.97	0.47
1:B:230:THR:HG21	1:B:298:HIS:ND1	2.28	0.47
1:C:38:ILE:HD11	1:C:107:LEU:CB	2.44	0.47
1:B:38:ILE:HD11	1:B:107:LEU:HB3	1.97	0.47
1:E:38:ILE:HD12	1:E:38:ILE:O	2.15	0.47
1:D:79:ASP:O	1:D:81:ARG:N	2.48	0.47
1:B:307:LEU:HB3	1:B:335:ALA:HB1	1.96	0.47
1:E:263:LEU:HG	1:E:264:PRO:CD	2.43	0.47
1:E:238:THR:C	1:E:240:MET:N	2.64	0.47
1:B:304:THR:HG22	1:B:305:ALA:N	2.30	0.47
1:D:317:ARG:NH2	2:R:4:A:O2'	2.47	0.47
1:C:408:ARG:HB3	2:R:15:A:N6	2.30	0.47
1:E:151:GLU:O	1:E:155:LYS:N	2.37	0.47
1:C:257:GLU:OE1	1:C:295:PRO:HD2	2.14	0.47
1:C:158:ASP:C	1:C:160:LEU:N	2.68	0.47
1:B:308:LEU:HD11	1:B:335:ALA:O	2.14	0.47
1:A:234:LEU:HD11	1:A:304:THR:CG2	2.45	0.47
1:D:18:LEU:HB2	1:D:19:PRO:HD2	1.96	0.47
1:B:150:PRO:N	1:B:152:TYR:CE1	2.83	0.47
1:C:43:ASN:ND2	1:C:113:LEU:N	2.62	0.47
1:C:316:ALA:HA	2:R:14:A:H5'	1.97	0.47
1:C:29:ALA:HB3	1:C:266:GLN:OE1	2.15	0.47
1:E:253:GLU:CD	1:E:253:GLU:N	2.62	0.47
1:E:390:THR:O	1:E:393:MET:HG2	2.14	0.47
1:B:323:GLU:OE2	1:C:373:ARG:NH2	2.44	0.47
1:E:87:ASP:O	1:E:88:TRP:HB2	2.15	0.47
1:C:148:GLN:C	1:C:152:TYR:CE2	2.88	0.47
1:A:128:SER:CA	1:A:130:ASP:HB2	2.38	0.47
1:D:106:ASP:C	1:D:107:LEU:HD12	2.35	0.47
1:A:172:GLU:CB	1:A:173:PRO:CD	2.92	0.47
1:C:40:LEU:HD22	1:C:42:ILE:HG13	1.97	0.47
1:C:383:GLU:HG2	1:C:387:ARG:HD3	1.97	0.47
1:A:328:THR:CG2	1:A:415:TYR:CE1	2.95	0.47
1:C:91:PHE:CZ	1:C:267:GLU:HG3	2.50	0.47
1:D:174:LEU:N	1:D:174:LEU:HD12	2.29	0.47
1:D:9:ILE:CG2	1:D:10:ASP:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASN:O	1:A:111:LYS:HG3	2.15	0.46
1:B:149:MET:HG3	2:R:24:A:N9	2.30	0.46
1:A:38:ILE:HD11	1:A:107:LEU:CB	2.45	0.46
1:E:52:ARG:HE	1:E:130:ASP:CG	2.17	0.46
1:B:31:TYR:C	1:B:31:TYR:CD1	2.88	0.46
1:D:46:LYS:O	1:D:47:SER:O	2.34	0.46
1:C:148:GLN:CD	1:C:179:ARG:HE	2.17	0.46
1:E:150:PRO:N	1:E:152:TYR:CZ	2.83	0.46
1:E:177:GLU:HB3	1:E:178:GLY:H	1.47	0.46
1:C:313:ALA:O	1:C:314:ARG:C	2.53	0.46
1:C:314:ARG:O	1:C:413:GLY:HA3	2.15	0.46
1:C:38:ILE:HD11	1:C:107:LEU:HB3	1.97	0.46
1:C:165:LYS:C	1:C:167:ILE:HG12	2.35	0.46
1:C:40:LEU:HD11	1:C:194:ILE:HG12	1.96	0.46
1:C:336:TYR:O	1:C:337:ALA:C	2.54	0.46
1:A:269:ASP:HB3	1:E:17:LYS:HB2	1.97	0.46
1:D:83:LYS:HD2	1:D:83:LYS:N	2.31	0.46
1:E:83:LYS:N	1:E:83:LYS:HD2	2.30	0.46
1:E:149:MET:CG	2:R:42:A:C1'	2.91	0.46
1:A:31:TYR:CD1	1:A:31:TYR:C	2.87	0.46
1:D:143:ARG:HE	1:D:155:LYS:HE2	1.80	0.46
2:R:9:A:H2'	2:R:10:A:O4'	2.15	0.46
1:A:177:GLU:HA	1:A:181:ILE:CD1	2.36	0.46
1:A:177:GLU:OE1	1:A:183:ASP:OD1	2.33	0.46
1:A:224:ASP:CG	2:R:30:A:H4'	2.36	0.46
1:D:199:ASP:OD1	1:D:214:ARG:HD2	2.16	0.46
1:C:177:GLU:OE1	1:C:183:ASP:OD1	2.33	0.46
1:A:44:THR:HG22	1:A:46:LYS:HZ2	1.73	0.46
1:E:328:THR:HG21	1:E:415:TYR:HE1	1.77	0.46
1:B:325:THR:CG2	1:C:309:ARG:HH11	2.28	0.46
1:C:263:LEU:HG	1:C:264:PRO:CD	2.45	0.46
1:B:91:PHE:CZ	1:B:267:GLU:HG3	2.51	0.46
1:B:27:TYR:HB3	1:B:266:GLN:HE22	1.78	0.46
1:D:149:MET:C	1:D:152:TYR:CE1	2.89	0.46
1:E:149:MET:C	1:E:152:TYR:CE1	2.88	0.46
1:A:106:ASP:C	1:A:107:LEU:HD12	2.36	0.46
1:A:29:ALA:HB3	1:A:266:GLN:OE1	2.16	0.46
1:C:160:LEU:C	1:C:160:LEU:HD12	2.35	0.46
1:A:98:ALA:C	1:A:100:ASP:H	2.18	0.46
1:E:369:PRO:HA	1:E:370:PRO:HD3	1.81	0.46
1:B:47:SER:HB3	1:B:50:ASP:CB	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ARG:NH2	1:B:176:PRO:O	2.49	0.46
1:C:408:ARG:HD3	2:R:15:A:C5	2.51	0.46
1:B:298:HIS:NE2	1:B:317:ARG:NH1	2.64	0.46
1:C:250:LEU:HD13	1:D:344:LEU:CD1	2.41	0.46
1:B:235:CYS:HA	1:B:245:VAL:HG21	1.97	0.46
1:C:228:LEU:HD11	1:C:268:ILE:HG22	1.98	0.46
1:B:83:LYS:N	1:B:83:LYS:HD2	2.31	0.46
1:C:83:LYS:HD2	1:C:83:LYS:N	2.31	0.46
1:D:313:ALA:O	1:D:315:ASN:N	2.48	0.46
1:A:148:GLN:C	1:A:152:TYR:CE2	2.90	0.46
1:B:408:ARG:HD3	2:R:24:A:N6	2.31	0.46
1:C:149:MET:C	1:C:152:TYR:CE1	2.89	0.46
1:B:314:ARG:O	1:B:413:GLY:HA3	2.16	0.46
1:B:133:TRP:O	1:B:136:LEU:N	2.49	0.46
1:B:308:LEU:O	1:B:309:ARG:HB2	2.15	0.46
1:A:243:GLU:O	1:A:247:THR:HG23	2.16	0.46
1:C:323:GLU:OE2	1:D:373:ARG:NH2	2.42	0.46
1:B:247:THR:HA	1:C:348:PHE:HB2	1.96	0.46
1:A:83:LYS:HD2	1:A:83:LYS:N	2.31	0.46
1:D:261:MET:HB3	1:D:262:MET:HE3	1.97	0.46
1:E:199:ASP:CB	1:E:217:THR:HG23	2.46	0.46
1:E:148:GLN:C	1:E:152:TYR:CE2	2.90	0.46
1:E:152:TYR:HD1	1:E:153:ARG:N	2.05	0.46
1:B:316:ALA:HB1	1:B:317:ARG:HH22	1.80	0.46
1:D:38:ILE:HD11	1:D:107:LEU:HB3	1.98	0.46
1:D:37:GLU:O	1:D:39:PRO:HD3	2.15	0.46
1:C:336:TYR:CD1	1:C:393:MET:HB3	2.51	0.46
1:B:342:ALA:CB	1:B:344:LEU:HD23	2.45	0.46
2:R:4:A:H8	2:R:4:A:O5'	1.99	0.46
1:A:143:ARG:HE	1:A:155:LYS:HE2	1.81	0.46
1:E:46:LYS:O	1:E:47:SER:O	2.34	0.46
1:B:148:GLN:CD	1:B:179:ARG:HE	2.17	0.46
1:C:177:GLU:CA	1:C:181:ILE:HD11	2.33	0.46
1:D:42:ILE:HD12	1:D:74:TYR:HD2	1.81	0.46
1:E:79:ASP:O	1:E:79:ASP:CG	2.54	0.46
1:E:278:LEU:HD23	1:E:279:ILE:N	2.30	0.46
1:D:279:ILE:HD11	1:D:287:SER:HB3	1.98	0.46
1:C:401:VAL:HG21	1:C:420:PHE:HB2	1.98	0.46
1:A:104:ILE:HG22	1:A:104:ILE:O	2.15	0.46
1:A:7:ARG:NH1	1:B:259:VAL:HG21	2.31	0.46
1:A:212:SER:HA	2:R:36:A:N3	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:O	1:B:49:SER:C	2.53	0.46
1:D:153:ARG:NH2	1:D:176:PRO:O	2.49	0.45
1:D:44:THR:HA	1:D:46:LYS:HE3	1.94	0.45
1:C:152:TYR:HD1	1:C:153:ARG:N	2.08	0.45
1:A:165:LYS:O	1:A:167:ILE:N	2.48	0.45
1:A:107:LEU:H	1:A:107:LEU:HD12	1.75	0.45
1:D:38:ILE:O	1:D:38:ILE:HD12	2.16	0.45
1:C:320:ASP:HA	1:C:324:TYR:HH	1.80	0.45
2:R:1:A:C2'	2:R:2:A:H5'	2.46	0.45
1:C:323:GLU:O	1:C:327:LEU:HD22	2.16	0.45
1:D:149:MET:C	1:D:152:TYR:CE2	2.89	0.45
1:D:151:GLU:O	1:D:155:LYS:HB2	2.15	0.45
1:D:177:GLU:OE1	1:D:183:ASP:OD1	2.34	0.45
1:D:317:ARG:HH21	2:R:4:A:C2'	2.28	0.45
2:R:5:A:N6	2:R:7:A:C2	2.84	0.45
1:E:148:GLN:NE2	1:E:179:ARG:NE	2.60	0.45
1:E:150:PRO:HA	1:E:152:TYR:CD1	2.51	0.45
1:A:38:ILE:HD11	1:A:107:LEU:HB3	1.99	0.45
1:B:37:GLU:O	1:B:39:PRO:HD3	2.16	0.45
1:C:376:VAL:HG22	1:D:346:GLN:OE1	2.16	0.45
1:D:383:GLU:HG2	1:D:387:ARG:HD3	1.99	0.45
1:A:84:LEU:HD21	1:A:88:TRP:HE3	1.79	0.45
1:C:48:LEU:O	1:C:49:SER:C	2.54	0.45
2:R:29:A:C2'	2:R:30:A:H5"	2.47	0.45
1:B:177:GLU:OE1	1:B:183:ASP:OD1	2.33	0.45
1:E:148:GLN:CD	1:E:179:ARG:HE	2.19	0.45
1:C:105:PHE:C	1:C:107:LEU:N	2.66	0.45
1:D:38:ILE:HD11	1:D:107:LEU:CB	2.46	0.45
1:A:27:TYR:HB3	1:A:266:GLN:HE22	1.78	0.45
1:B:250:LEU:HD22	1:B:379:LEU:HD21	1.98	0.45
1:A:309:ARG:HG2	1:E:415:TYR:CE2	2.50	0.45
1:B:79:ASP:O	1:B:79:ASP:CG	2.53	0.45
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.82	0.45
1:B:401:VAL:HG21	1:B:420:PHE:HB2	1.98	0.45
1:C:327:LEU:HA	1:C:327:LEU:HD12	1.79	0.45
1:A:2:SER:O	1:B:243:GLU:HG3	2.17	0.45
1:C:235:CYS:HA	1:C:245:VAL:HG21	1.97	0.45
1:E:248:TRP:HZ3	1:E:333:LEU:HD23	1.81	0.45
1:B:388:LYS:HB2	1:B:388:LYS:HE3	1.83	0.45
1:E:199:ASP:HB2	1:E:217:THR:HG23	1.97	0.45
1:B:408:ARG:HB3	2:R:24:A:N6	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LEU:HA	1:B:141:LEU:HD12	1.98	0.45
1:B:380:GLY:N	1:C:354:LYS:HD2	2.31	0.45
1:A:320:ASP:HA	1:A:324:TYR:HH	1.80	0.45
1:E:268:ILE:H	1:E:268:ILE:HG12	1.32	0.45
1:E:251:ASN:O	1:E:252:ARG:C	2.55	0.45
1:B:121:VAL:HG12	1:B:121:VAL:O	2.16	0.45
1:B:43:ASN:CG	1:B:112:ALA:HB3	2.35	0.45
1:E:170:GLN:HG3	1:E:171:PHE:HB3	1.98	0.45
1:C:149:MET:C	1:C:152:TYR:CE2	2.90	0.45
1:A:72:TYR:HE1	1:A:134:LEU:HD12	1.77	0.45
1:B:136:LEU:HD13	1:B:163:GLN:HG3	1.99	0.45
1:B:29:ALA:HB3	1:B:266:GLN:OE1	2.16	0.45
1:A:263:LEU:HG	1:A:264:PRO:CD	2.46	0.45
1:B:263:LEU:HG	1:B:264:PRO:CD	2.46	0.45
1:D:336:TYR:CE2	1:D:340:SER:HB3	2.52	0.45
1:B:268:ILE:HG12	1:B:268:ILE:H	1.36	0.45
1:C:243:GLU:O	1:C:247:THR:HG23	2.17	0.45
1:D:7:ARG:O	1:D:11:ASN:HA	2.16	0.45
1:B:46:LYS:O	1:B:47:SER:O	2.35	0.45
1:C:150:PRO:N	1:C:152:TYR:CZ	2.85	0.45
1:C:163:GLN:N	1:C:163:GLN:CD	2.70	0.45
1:E:200:MET:HB2	1:E:277:TYR:CE2	2.52	0.45
1:A:148:GLN:CD	1:A:179:ARG:HE	2.20	0.45
2:R:29:A:H2'	2:R:30:A:C5'	2.47	0.45
1:A:408:ARG:HD3	2:R:33:A:C5	2.52	0.45
1:C:46:LYS:O	1:C:47:SER:O	2.35	0.45
1:E:136:LEU:HD13	1:E:163:GLN:HG3	1.98	0.45
1:E:383:GLU:HG2	1:E:387:ARG:HD3	1.98	0.45
1:B:407:LEU:HD13	1:B:413:GLY:C	2.37	0.45
1:C:312:ARG:HG3	2:R:14:A:C4	2.52	0.45
1:A:44:THR:HA	1:A:46:LYS:CE	2.46	0.45
1:B:165:LYS:H	1:B:167:ILE:HD12	1.82	0.45
1:B:9:ILE:CG2	1:B:10:ASP:H	2.23	0.45
1:D:29:ALA:C	1:D:31:TYR:N	2.69	0.45
2:R:8:A:H2'	2:R:9:A:H5"	1.99	0.45
1:B:74:TYR:O	1:B:78:LYS:HD3	2.17	0.45
1:E:163:GLN:CD	1:E:163:GLN:N	2.70	0.45
1:E:160:LEU:HD22	1:E:171:PHE:HB2	1.98	0.45
1:B:148:GLN:C	1:B:152:TYR:CE2	2.90	0.45
1:E:408:ARG:HB3	2:R:42:A:N6	2.31	0.45
1:E:81:ARG:CB	1:E:208:HIS:HE2	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:HG21	1:E:7:ARG:HH11	1.81	0.45
1:A:307:LEU:HB3	1:A:335:ALA:HB1	1.99	0.45
1:C:215:TYR:HA	2:R:18:A:O4'	2.17	0.45
1:E:104:ILE:CG2	1:E:104:ILE:O	2.65	0.45
1:C:326:SER:HB3	1:D:343:ASP:HB2	1.99	0.45
1:D:247:THR:OG1	1:D:375:VAL:HG21	2.16	0.45
1:D:149:MET:O	1:D:152:TYR:CD2	2.70	0.45
1:D:143:ARG:NH2	2:R:9:A:OP2	2.47	0.45
1:D:79:ASP:CG	1:D:79:ASP:O	2.53	0.45
1:D:264:PRO:O	1:D:266:GLN:HG2	2.17	0.45
1:D:336:TYR:O	1:D:337:ALA:C	2.54	0.45
1:C:41:TYR:HB2	1:C:190:ASN:HD21	1.82	0.45
1:D:243:GLU:O	1:D:247:THR:HG23	2.17	0.45
1:A:117:LEU:CB	1:A:118:PRO:CD	2.86	0.45
1:C:149:MET:HG3	2:R:15:A:N9	2.32	0.45
2:R:22:A:OP2	2:R:22:A:H8	2.00	0.45
1:B:158:ASP:HA	1:B:161:THR:HG23	1.99	0.45
1:D:138:LEU:HA	1:D:141:LEU:HD12	1.99	0.45
1:C:87:ASP:O	1:C:88:TRP:HB2	2.18	0.45
1:B:234:LEU:HD11	1:B:304:THR:CG2	2.47	0.45
1:D:233:HIS:O	1:D:237:ILE:HB	2.17	0.45
1:A:107:LEU:CD1	1:A:107:LEU:N	2.64	0.44
1:D:299:PHE:HZ	1:D:415:TYR:CE1	2.35	0.44
1:A:323:GLU:OE1	1:B:239:GLY:HA3	2.17	0.44
1:A:91:PHE:CZ	1:A:267:GLU:HG3	2.52	0.44
1:B:313:ALA:O	1:B:314:ARG:C	2.55	0.44
1:B:107:LEU:N	1:B:107:LEU:CD1	2.67	0.44
1:B:54:TYR:CD1	1:B:122:SER:HB2	2.53	0.44
1:B:228:LEU:HD11	1:B:268:ILE:HG22	2.00	0.44
1:E:48:LEU:O	1:E:49:SER:C	2.54	0.44
1:B:149:MET:CG	2:R:24:A:H1'	2.47	0.44
1:B:54:TYR:HD1	1:B:122:SER:HB2	1.83	0.44
1:B:223:LYS:O	1:B:224:ASP:HB2	2.18	0.44
1:C:15:VAL:HB	1:C:17:LYS:HZ3	1.82	0.44
1:A:138:LEU:HA	1:A:141:LEU:HD12	2.00	0.44
1:C:231:PHE:CE2	1:C:258:MET:HE1	2.52	0.44
1:E:275:MET:N	1:E:276:PRO:CD	2.80	0.44
1:C:44:THR:C	1:C:46:LYS:H	2.21	0.44
1:B:199:ASP:CB	1:B:217:THR:HG23	2.46	0.44
1:C:407:LEU:HD13	1:C:413:GLY:C	2.38	0.44
1:B:383:GLU:HG2	1:B:387:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:TYR:C	1:E:31:TYR:CD1	2.91	0.44
1:B:336:TYR:O	1:B:337:ALA:C	2.56	0.44
1:C:13:VAL:HG12	1:C:14:ILE:H	1.80	0.44
1:A:232:GLY:HA2	1:E:18:LEU:CD1	2.47	0.44
1:C:153:ARG:NH2	1:C:176:PRO:O	2.51	0.44
1:A:163:GLN:CD	1:A:163:GLN:N	2.71	0.44
1:E:314:ARG:O	1:E:413:GLY:HA3	2.17	0.44
1:A:52:ARG:HE	1:A:130:ASP:CG	2.19	0.44
1:E:190:ASN:O	1:E:194:ILE:HG13	2.17	0.44
1:E:40:LEU:HD22	1:E:42:ILE:CG1	2.48	0.44
1:C:398:LYS:HD2	1:C:421:ASP:HA	1.99	0.44
1:B:149:MET:O	1:B:152:TYR:CD1	2.71	0.44
1:C:149:MET:CA	1:C:152:TYR:CE2	3.01	0.44
1:E:45:THR:H	1:E:111:LYS:HE3	1.81	0.44
1:E:41:TYR:HB2	1:E:190:ASN:HD21	1.83	0.44
1:B:104:ILE:O	1:B:104:ILE:CG2	2.65	0.44
1:A:177:GLU:HB3	1:A:178:GLY:H	1.48	0.44
1:D:163:GLN:CD	1:D:163:GLN:N	2.71	0.44
1:E:149:MET:C	1:E:152:TYR:CE2	2.91	0.44
1:E:128:SER:CA	1:E:130:ASP:HB2	2.40	0.44
1:B:251:ASN:O	1:B:252:ARG:C	2.55	0.44
1:E:78:LYS:O	1:E:80:ILE:N	2.51	0.44
1:A:121:VAL:O	1:A:121:VAL:HG12	2.17	0.44
1:E:138:LEU:HA	1:E:141:LEU:HD12	2.00	0.44
1:D:44:THR:HG23	1:D:116:VAL:HG11	2.00	0.44
1:E:177:GLU:OE1	1:E:183:ASP:OD1	2.36	0.44
1:B:379:LEU:HB3	1:C:354:LYS:CD	2.48	0.44
1:C:81:ARG:CB	1:C:208:HIS:HE2	2.31	0.44
1:A:273:SER:OG	1:A:274:TYR:N	2.50	0.44
1:E:273:SER:OG	1:E:274:TYR:N	2.51	0.44
1:C:202:PHE:CD2	1:C:211:ALA:HA	2.53	0.44
1:D:222:PHE:HB3	1:D:225:CYS:HB2	2.00	0.44
1:D:327:LEU:HD12	1:D:327:LEU:HA	1.79	0.44
1:B:195:VAL:CG2	1:B:196:ALA:N	2.81	0.44
1:E:233:HIS:O	1:E:237:ILE:HB	2.18	0.44
1:D:44:THR:C	1:D:46:LYS:H	2.21	0.44
1:E:149:MET:CA	1:E:152:TYR:CE2	3.01	0.44
1:C:79:ASP:O	1:C:79:ASP:CG	2.55	0.44
1:A:327:LEU:HD12	1:A:327:LEU:HA	1.76	0.44
1:B:248:TRP:HZ3	1:B:333:LEU:HD23	1.83	0.44
1:D:234:LEU:HD11	1:D:304:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASP:CG	1:B:33:ARG:HH21	2.20	0.44
1:A:154:LYS:HE3	1:A:154:LYS:HB2	1.87	0.44
1:D:314:ARG:O	1:D:413:GLY:HA3	2.18	0.43
1:A:178:GLY:O	1:A:179:ARG:C	2.57	0.43
1:E:230:THR:HG21	1:E:298:HIS:ND1	2.33	0.43
1:B:163:GLN:HA	1:B:167:ILE:HD13	2.00	0.43
1:E:106:ASP:C	1:E:107:LEU:HD12	2.38	0.43
1:A:79:ASP:CG	1:A:79:ASP:O	2.56	0.43
1:C:74:TYR:O	1:C:78:LYS:HD3	2.18	0.43
1:A:299:PHE:HZ	1:A:415:TYR:CE1	2.36	0.43
1:D:181:ILE:CD1	1:D:181:ILE:H	2.18	0.43
1:D:408:ARG:HB3	2:R:6:A:N6	2.33	0.43
1:B:42:ILE:O	1:B:111:LYS:HA	2.18	0.43
1:C:199:ASP:HB2	1:C:217:THR:HG23	1.99	0.43
1:B:87:ASP:O	1:B:88:TRP:HB2	2.18	0.43
1:D:133:TRP:HD1	1:D:167:ILE:HD12	1.83	0.43
1:B:106:ASP:C	1:B:107:LEU:HD12	2.37	0.43
1:E:234:LEU:HD11	1:E:304:THR:CG2	2.49	0.43
1:C:2:SER:O	1:D:243:GLU:HG3	2.18	0.43
1:A:261:MET:HB3	1:A:262:MET:HE3	1.99	0.43
1:D:121:VAL:O	1:D:121:VAL:HG12	2.18	0.43
1:A:407:LEU:HD13	1:A:413:GLY:C	2.39	0.43
1:D:149:MET:CA	1:D:152:TYR:CE2	3.01	0.43
1:A:153:ARG:NH2	1:A:176:PRO:O	2.51	0.43
1:B:199:ASP:OD1	1:B:214:ARG:HD2	2.17	0.43
1:C:137:TYR:OH	1:C:172:GLU:HB3	2.18	0.43
1:D:98:ALA:C	1:D:100:ASP:N	2.70	0.43
1:B:181:ILE:H	1:B:181:ILE:CD1	2.08	0.43
1:E:408:ARG:NH2	2:R:43:A:OP1	2.31	0.43
1:B:163:GLN:N	1:B:163:GLN:CD	2.72	0.43
1:C:134:LEU:HD13	1:C:134:LEU:O	2.18	0.43
1:E:52:ARG:NH2	1:E:130:ASP:OD2	2.42	0.43
1:D:37:GLU:HB2	1:D:108:VAL:CG1	2.44	0.43
1:A:374:ASP:OD1	1:A:376:VAL:N	2.50	0.43
1:C:74:TYR:CE1	1:C:78:LYS:HD2	2.53	0.43
1:D:228:LEU:HD11	1:D:268:ILE:HG22	2.00	0.43
1:E:288:PRO:HG2	1:E:289:TYR:CE2	2.54	0.43
1:D:109:SER:O	1:D:110:LEU:HD23	2.19	0.43
1:C:84:LEU:HD21	1:C:88:TRP:HE3	1.83	0.43
1:B:174:LEU:N	1:B:174:LEU:HD23	2.34	0.43
1:B:42:ILE:HD12	1:B:74:TYR:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:H	1:B:111:LYS:HE3	1.83	0.43
1:E:313:ALA:O	1:E:315:ASN:N	2.51	0.43
1:E:407:LEU:HD13	1:E:413:GLY:C	2.39	0.43
1:C:387:ARG:HB3	1:C:387:ARG:CZ	2.48	0.43
1:B:240:MET:HE2	1:B:245:VAL:HA	2.00	0.43
1:B:270:LYS:HB3	1:B:273:SER:HB2	1.99	0.43
1:C:121:VAL:O	1:C:121:VAL:HG12	2.17	0.43
1:E:119:ASP:OD1	1:E:119:ASP:N	2.51	0.43
1:D:195:VAL:CG2	1:D:196:ALA:N	2.82	0.43
1:A:148:GLN:NE2	1:A:179:ARG:NE	2.60	0.43
1:A:152:TYR:HD1	1:A:153:ARG:N	2.09	0.43
1:B:151:GLU:O	1:B:155:LYS:HB2	2.18	0.43
1:E:303:LEU:HD22	1:E:328:THR:HG22	1.99	0.43
1:A:336:TYR:CE1	1:A:393:MET:HB3	2.54	0.43
1:E:342:ALA:HB3	1:E:344:LEU:HD23	2.00	0.43
1:B:180:ASP:OD2	1:C:164:CYS:HB3	2.19	0.43
1:E:137:TYR:OH	1:E:172:GLU:HB3	2.19	0.43
1:E:166:MET:C	1:E:167:ILE:HG13	2.39	0.43
1:B:44:THR:HG23	1:B:116:VAL:HG11	2.00	0.43
1:A:133:TRP:HB3	1:A:167:ILE:HD13	1.99	0.43
1:C:29:ALA:C	1:C:31:TYR:N	2.70	0.43
1:A:52:ARG:NH2	1:A:130:ASP:OD2	2.41	0.43
1:C:268:ILE:H	1:C:268:ILE:HG12	1.34	0.43
1:C:234:LEU:HD11	1:C:304:THR:CG2	2.49	0.43
1:D:230:THR:HG21	1:D:298:HIS:ND1	2.33	0.43
1:A:151:GLU:O	1:A:155:LYS:HB2	2.19	0.43
1:A:279:ILE:HD11	1:A:287:SER:CB	2.48	0.43
1:B:141:LEU:HD23	1:B:182:PHE:CZ	2.53	0.43
1:A:81:ARG:CB	1:A:208:HIS:HE2	2.30	0.43
1:A:119:ASP:OD1	1:A:119:ASP:N	2.51	0.43
1:B:40:LEU:HD11	1:B:194:ILE:HG12	2.00	0.43
1:B:128:SER:CA	1:B:130:ASP:HB2	2.40	0.43
1:D:74:TYR:O	1:D:78:LYS:HD3	2.18	0.43
1:A:79:ASP:O	1:A:81:ARG:N	2.51	0.43
1:A:309:ARG:HD2	1:E:325:THR:HG23	2.01	0.43
1:D:387:ARG:HH11	1:D:387:ARG:HB3	1.84	0.43
1:C:123:ASP:C	1:C:125:SER:H	2.21	0.43
1:E:84:LEU:HD21	1:E:88:TRP:HE3	1.83	0.43
1:D:150:PRO:N	1:D:152:TYR:CZ	2.87	0.43
1:E:133:TRP:O	1:E:136:LEU:N	2.52	0.43
1:E:44:THR:HA	1:E:46:LYS:HE3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:C	1:B:152:TYR:CE2	2.92	0.43
1:D:387:ARG:HB3	1:D:387:ARG:CZ	2.48	0.43
1:B:220:SER:HG	1:B:277:TYR:HD1	1.65	0.43
1:C:195:VAL:CG2	1:C:196:ALA:N	2.81	0.43
1:D:150:PRO:HA	1:D:152:TYR:CD1	2.53	0.43
1:A:364:LEU:O	1:A:366:THR:N	2.45	0.43
1:D:74:TYR:CD1	1:D:78:LYS:HD2	2.53	0.43
1:B:303:LEU:O	1:B:307:LEU:HD22	2.19	0.43
1:E:174:LEU:N	1:E:174:LEU:CD1	2.81	0.43
1:D:97:LYS:O	1:D:99:GLY:N	2.52	0.42
1:B:177:GLU:HB3	1:B:178:GLY:H	1.46	0.42
1:A:133:TRP:O	1:A:136:LEU:N	2.52	0.42
1:B:163:GLN:C	1:B:167:ILE:HD13	2.40	0.42
1:D:74:TYR:CE1	1:D:78:LYS:HD2	2.53	0.42
1:A:240:MET:HE2	1:A:245:VAL:HA	2.00	0.42
1:E:299:PHE:HZ	1:E:415:TYR:CE1	2.37	0.42
1:C:104:ILE:HG12	1:C:201:PHE:CD1	2.54	0.42
1:C:344:LEU:O	1:C:345:ALA:HB2	2.18	0.42
1:C:388:LYS:HB2	1:C:388:LYS:HE3	1.84	0.42
1:D:286:LYS:HD2	2:R:3:A:OP2	2.19	0.42
1:E:44:THR:C	1:E:46:LYS:H	2.22	0.42
1:C:136:LEU:HD13	1:C:163:GLN:HG3	2.01	0.42
1:C:74:TYR:CD1	1:C:78:LYS:HD2	2.53	0.42
1:C:104:ILE:CG2	1:C:104:ILE:O	2.67	0.42
1:C:32:PHE:HA	1:C:35:SER:O	2.19	0.42
1:A:174:LEU:N	1:A:174:LEU:HD23	2.34	0.42
1:D:48:LEU:O	1:D:49:SER:C	2.56	0.42
1:E:387:ARG:HB3	1:E:387:ARG:CZ	2.48	0.42
1:D:107:LEU:CD1	1:D:107:LEU:N	2.67	0.42
1:E:308:LEU:O	1:E:309:ARG:HB2	2.19	0.42
1:D:223:LYS:O	1:D:224:ASP:HB2	2.18	0.42
1:C:59:LEU:C	1:C:61:SER:N	2.71	0.42
1:B:320:ASP:HA	1:B:324:TYR:HH	1.85	0.42
1:B:344:LEU:HA	1:B:344:LEU:HD13	1.82	0.42
1:B:119:ASP:N	1:B:119:ASP:OD1	2.52	0.42
1:A:149:MET:O	1:A:152:TYR:CD1	2.72	0.42
1:B:150:PRO:HA	1:B:152:TYR:CD1	2.54	0.42
2:R:26:A:C3'	2:R:26:A:C8	3.02	0.42
1:C:149:MET:HG3	2:R:15:A:C1'	2.48	0.42
1:D:344:LEU:O	1:D:345:ALA:HB2	2.18	0.42
1:C:79:ASP:O	1:C:81:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:THR:O	1:A:393:MET:HG2	2.19	0.42
1:D:104:ILE:O	1:D:104:ILE:CG2	2.66	0.42
1:D:248:TRP:HZ3	1:D:333:LEU:HD23	1.84	0.42
1:E:79:ASP:O	1:E:81:ARG:N	2.52	0.42
1:C:308:LEU:HD11	1:C:335:ALA:O	2.19	0.42
1:D:29:ALA:HB3	1:D:266:GLN:OE1	2.19	0.42
1:D:288:PRO:HG2	1:D:289:TYR:CE2	2.54	0.42
1:B:243:GLU:O	1:B:247:THR:HG23	2.19	0.42
1:D:323:GLU:O	1:D:327:LEU:HD22	2.19	0.42
1:D:250:LEU:HD22	1:D:379:LEU:HD21	2.02	0.42
1:A:223:LYS:O	1:A:224:ASP:HB2	2.20	0.42
1:E:163:GLN:O	1:E:167:ILE:HB	2.20	0.42
1:B:44:THR:C	1:B:46:LYS:H	2.23	0.42
1:B:151:GLU:O	1:B:155:LYS:N	2.37	0.42
1:C:317:ARG:CZ	2:R:13:A:O2'	2.67	0.42
1:E:295:PRO:HB2	1:E:322:ILE:HG21	2.02	0.42
1:B:327:LEU:HA	1:B:327:LEU:HD12	1.87	0.42
1:C:231:PHE:CZ	1:C:258:MET:CE	3.02	0.42
1:A:407:LEU:HA	1:A:407:LEU:HD23	1.79	0.42
1:A:174:LEU:CD2	1:A:174:LEU:N	2.83	0.42
1:D:317:ARG:NE	2:R:4:A:O2'	2.48	0.42
1:D:317:ARG:CZ	2:R:4:A:C2'	2.97	0.42
1:D:408:ARG:HD3	2:R:6:A:C5	2.54	0.42
1:C:45:THR:H	1:C:111:LYS:HE3	1.83	0.42
1:C:279:ILE:HD11	1:C:287:SER:HB3	2.01	0.42
1:E:9:ILE:CG2	1:E:10:ASP:N	2.81	0.42
1:D:81:ARG:CB	1:D:208:HIS:HE2	2.30	0.42
1:C:307:LEU:HB3	1:C:335:ALA:HB1	2.01	0.42
1:D:240:MET:HE2	1:D:245:VAL:HA	2.02	0.42
1:A:7:ARG:NH2	1:B:256:ASP:OD2	2.50	0.42
1:C:245:VAL:HG22	1:C:334:TYR:OH	2.20	0.42
1:D:166:MET:O	1:D:167:ILE:CD1	2.65	0.42
1:B:177:GLU:HA	1:B:181:ILE:CD1	2.32	0.42
1:A:295:PRO:HB2	1:A:322:ILE:HG21	2.01	0.42
1:B:128:SER:C	1:B:130:ASP:N	2.73	0.42
1:B:29:ALA:C	1:B:31:TYR:N	2.70	0.42
1:A:218:ILE:C	1:A:220:SER:H	2.22	0.42
1:C:248:TRP:HZ3	1:C:333:LEU:HD23	1.85	0.42
2:R:32:A:H5"	2:R:33:A:OP1	2.19	0.42
1:D:133:TRP:CD1	1:D:167:ILE:HD12	2.55	0.42
1:C:143:ARG:NE	1:C:155:LYS:HE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:ILE:H	1:E:181:ILE:CD1	2.10	0.42
2:R:42:A:H5"	2:R:43:A:C5'	2.50	0.42
1:B:107:LEU:H	1:B:107:LEU:HD12	1.80	0.42
1:C:8:ILE:HG13	1:C:9:ILE:N	2.35	0.42
1:B:79:ASP:O	1:B:81:ARG:N	2.53	0.42
1:B:287:SER:HA	1:B:288:PRO:HD2	1.89	0.42
1:E:15:VAL:HB	1:E:17:LYS:HZ3	1.84	0.42
1:A:87:ASP:O	1:A:88:TRP:HB2	2.18	0.42
1:B:261:MET:HB3	1:B:262:MET:HE3	2.01	0.42
1:E:345:ALA:O	1:E:346:GLN:C	2.57	0.42
1:A:48:LEU:O	1:A:49:SER:C	2.57	0.42
1:D:179:ARG:HA	1:D:183:ASP:CG	2.40	0.42
1:C:278:LEU:HD23	1:C:279:ILE:N	2.34	0.42
1:B:163:GLN:CA	1:B:167:ILE:HD13	2.50	0.42
1:D:295:PRO:HB2	1:D:322:ILE:HG21	2.02	0.42
1:A:66:ILE:HD11	1:A:191:TYR:HB2	2.02	0.42
1:D:279:ILE:HD11	1:D:287:SER:CB	2.50	0.42
1:C:390:THR:HA	1:C:391:PRO:HD2	1.85	0.42
1:D:251:ASN:O	1:D:252:ARG:C	2.58	0.42
1:D:90:SER:O	1:D:91:PHE:HB2	2.19	0.42
1:D:202:PHE:CD2	1:D:211:ALA:HA	2.55	0.42
1:D:307:LEU:HB3	1:D:335:ALA:HB1	2.01	0.42
1:C:251:ASN:O	1:C:252:ARG:C	2.58	0.42
1:D:32:PHE:HA	1:D:35:SER:O	2.20	0.42
1:C:164:CYS:HA	1:C:168:ASN:CA	2.16	0.41
1:D:199:ASP:HB2	1:D:217:THR:HG23	2.01	0.41
1:E:153:ARG:CZ	1:E:176:PRO:C	2.88	0.41
1:A:344:LEU:HD12	1:E:250:LEU:HD13	2.02	0.41
1:C:78:LYS:O	1:C:80:ILE:N	2.52	0.41
1:B:279:ILE:HD11	1:B:287:SER:HB3	2.02	0.41
1:A:358:ASP:O	1:A:360:SER:N	2.53	0.41
1:A:104:ILE:HG12	1:A:201:PHE:CD1	2.55	0.41
1:A:7:ARG:HH11	1:B:259:VAL:HG21	1.85	0.41
2:R:45:A:O4'	2:R:45:A:N3	2.53	0.41
1:B:231:PHE:CE2	1:B:258:MET:HE1	2.55	0.41
1:D:369:PRO:HA	1:D:370:PRO:HD3	1.80	0.41
2:R:33:A:H5"	2:R:34:A:O5'	2.20	0.41
1:B:290:SER:HA	2:R:22:A:OP1	2.20	0.41
1:B:133:TRP:O	1:B:134:LEU:C	2.58	0.41
1:A:9:ILE:CG2	1:A:10:ASP:H	2.25	0.41
1:C:328:THR:HG21	1:C:415:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:LEU:HD12	1:E:327:LEU:HA	1.79	0.41
1:A:150:PRO:N	1:A:152:TYR:CZ	2.89	0.41
1:E:167:ILE:HG22	1:E:167:ILE:O	2.19	0.41
1:A:365:THR:CG2	1:A:366:THR:HG22	2.49	0.41
1:C:151:GLU:O	1:C:155:LYS:N	2.38	0.41
1:C:298:HIS:NE2	1:C:317:ARG:CZ	2.83	0.41
1:B:328:THR:HG22	1:B:415:TYR:HE1	1.85	0.41
1:C:328:THR:HG21	1:C:415:TYR:HE1	1.79	0.41
1:D:150:PRO:HD3	1:D:152:TYR:OH	2.20	0.41
1:B:295:PRO:HB2	1:B:322:ILE:HG21	2.01	0.41
1:C:295:PRO:HB2	1:C:322:ILE:HG21	2.02	0.41
1:C:292:VAL:HG11	2:R:12:A:H5"	1.96	0.41
1:B:81:ARG:CB	1:B:208:HIS:HE2	2.30	0.41
1:B:336:TYR:CE2	1:B:340:SER:HB3	2.55	0.41
1:B:398:LYS:HD2	1:B:421:ASP:HA	2.02	0.41
1:E:121:VAL:O	1:E:121:VAL:HG12	2.19	0.41
1:C:149:MET:O	1:C:152:TYR:N	2.44	0.41
1:E:322:ILE:HG12	1:E:324:TYR:CE2	2.56	0.41
1:A:180:ASP:OD2	1:B:164:CYS:HB3	2.20	0.41
1:A:387:ARG:CZ	1:A:387:ARG:HB3	2.50	0.41
1:D:287:SER:HA	1:D:288:PRO:HD2	1.91	0.41
1:C:398:LYS:O	1:C:402:MET:HG2	2.20	0.41
1:A:275:MET:N	1:A:276:PRO:CD	2.83	0.41
2:R:3:A:C6	2:R:4:A:N1	2.89	0.41
1:A:149:MET:C	1:A:152:TYR:CE1	2.94	0.41
2:R:30:A:H2'	2:R:31:A:C1'	2.50	0.41
1:C:199:ASP:CB	1:C:217:THR:HG23	2.50	0.41
1:D:84:LEU:HD23	1:D:84:LEU:HA	1.85	0.41
1:B:149:MET:CA	1:B:152:TYR:CE2	3.03	0.41
1:E:148:GLN:HA	1:E:148:GLN:OE1	2.20	0.41
1:E:387:ARG:HH11	1:E:387:ARG:HB3	1.82	0.41
1:C:230:THR:HG21	1:C:298:HIS:ND1	2.35	0.41
1:B:387:ARG:HB3	1:B:387:ARG:CZ	2.50	0.41
1:E:278:LEU:CD2	1:E:279:ILE:HG12	2.50	0.41
1:A:303:LEU:O	1:A:307:LEU:HD22	2.21	0.41
1:C:7:ARG:HH21	1:D:252:ARG:HD2	1.85	0.41
1:A:200:MET:HB2	1:A:277:TYR:CE2	2.55	0.41
1:A:195:VAL:CG2	1:A:196:ALA:N	2.83	0.41
1:B:64:VAL:O	1:B:64:VAL:HG13	2.19	0.41
1:B:84:LEU:HD21	1:B:88:TRP:HE3	1.84	0.41
1:D:133:TRP:O	1:D:136:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:C	1:B:152:TYR:CE1	2.93	0.41
1:A:342:ALA:CB	1:A:344:LEU:HD23	2.50	0.41
1:A:344:LEU:CD1	1:E:250:LEU:HD13	2.49	0.41
1:C:330:ALA:HA	1:D:344:LEU:HD11	2.02	0.41
1:D:40:LEU:HD11	1:D:194:ILE:HG12	2.02	0.41
1:E:328:THR:HG21	1:E:415:TYR:CZ	2.56	0.41
1:B:303:LEU:HD22	1:B:328:THR:HG22	2.03	0.41
1:D:308:LEU:O	1:D:309:ARG:HB2	2.20	0.41
1:C:213:PHE:C	1:C:215:TYR:H	2.22	0.41
1:A:200:MET:SD	1:A:274:TYR:CD2	3.14	0.41
1:D:234:LEU:HD11	1:D:304:THR:CG2	2.50	0.41
1:C:261:MET:HB3	1:C:262:MET:HE3	2.01	0.41
2:R:32:A:N6	2:R:34:A:C8	2.89	0.41
1:C:98:ALA:C	1:C:100:ASP:H	2.24	0.41
1:C:47:SER:HB3	1:C:50:ASP:CB	2.25	0.41
1:D:199:ASP:CB	1:D:217:THR:HG23	2.51	0.41
1:D:158:ASP:HA	1:D:161:THR:HG23	2.01	0.41
1:B:143:ARG:NE	1:B:155:LYS:HE2	2.35	0.41
1:C:181:ILE:HD12	1:C:183:ASP:OD2	2.21	0.41
1:C:183:ASP:OD2	1:C:183:ASP:N	2.54	0.41
1:D:66:ILE:HD11	1:D:191:TYR:HB2	2.03	0.41
1:E:365:THR:C	1:E:366:THR:HG22	2.41	0.41
1:E:336:TYR:CE2	1:E:340:SER:HB3	2.55	0.41
1:C:336:TYR:CE2	1:C:340:SER:HB3	2.56	0.41
1:C:228:LEU:HA	1:C:228:LEU:HD23	1.89	0.41
1:B:13:VAL:HG12	1:B:14:ILE:H	1.84	0.41
1:E:86:LYS:HB3	1:E:87:ASP:H	1.70	0.41
1:D:392:ASP:O	1:D:396:TYR:N	2.48	0.41
1:C:89:SER:O	1:C:90:SER:HB2	2.20	0.41
1:B:374:ASP:HB3	1:B:377:GLU:HB2	2.02	0.41
1:B:395:GLN:NE2	1:B:395:GLN:HA	2.34	0.41
1:E:388:LYS:HB2	1:E:388:LYS:HE3	1.88	0.41
1:B:202:PHE:CD2	1:B:211:ALA:HA	2.56	0.41
1:D:178:GLY:O	1:D:179:ARG:C	2.57	0.41
1:A:45:THR:H	1:A:111:LYS:HE3	1.84	0.41
1:E:143:ARG:NE	1:E:155:LYS:HE2	2.36	0.41
1:E:153:ARG:NH1	1:E:176:PRO:C	2.74	0.41
1:B:134:LEU:HD13	1:B:134:LEU:O	2.20	0.41
1:B:131:ASP:O	1:B:132:LYS:C	2.59	0.41
1:A:128:SER:C	1:A:130:ASP:N	2.74	0.41
1:C:128:SER:C	1:C:130:ASP:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:LEU:HD23	1:D:365:THR:N	2.36	0.41
1:B:15:VAL:HB	1:B:17:LYS:HZ3	1.86	0.41
1:D:303:LEU:HD22	1:D:328:THR:HG22	2.02	0.41
1:B:59:LEU:C	1:B:61:SER:N	2.72	0.41
1:C:288:PRO:HG2	1:C:289:TYR:CE2	2.56	0.41
1:A:220:SER:HG	1:A:277:TYR:HD1	1.68	0.41
1:B:273:SER:OG	1:B:274:TYR:N	2.53	0.41
1:C:119:ASP:OD1	1:C:119:ASP:N	2.52	0.41
1:E:154:LYS:HB2	1:E:154:LYS:HE3	1.86	0.41
1:D:374:ASP:OD1	1:D:376:VAL:N	2.51	0.41
1:A:149:MET:C	1:A:152:TYR:CE2	2.94	0.41
1:A:224:ASP:HA	2:R:30:A:O3'	2.21	0.41
1:E:158:ASP:HA	1:E:161:THR:HG23	2.03	0.41
1:E:27:TYR:HB3	1:E:266:GLN:HE22	1.83	0.41
1:E:308:LEU:HD13	1:E:308:LEU:N	2.36	0.41
1:D:245:VAL:HG22	1:D:334:TYR:OH	2.20	0.41
1:A:390:THR:HA	1:A:391:PRO:HD2	1.82	0.41
1:A:288:PRO:HG2	1:A:289:TYR:CE2	2.56	0.41
1:B:228:LEU:HA	1:B:228:LEU:HD23	1.89	0.41
1:E:44:THR:C	1:E:46:LYS:HD2	2.41	0.40
1:B:150:PRO:N	1:B:152:TYR:CZ	2.89	0.40
1:C:107:LEU:HD12	1:C:107:LEU:H	1.80	0.40
1:B:160:LEU:HD22	1:B:171:PHE:HB2	2.03	0.40
1:A:240:MET:HB3	1:A:240:MET:HE3	1.93	0.40
1:B:66:ILE:HD11	1:B:191:TYR:HB2	2.03	0.40
1:B:415:TYR:HE2	1:C:309:ARG:HG2	1.86	0.40
1:E:213:PHE:C	1:E:215:TYR:H	2.25	0.40
1:B:174:LEU:CD2	1:B:174:LEU:N	2.84	0.40
1:D:119:ASP:OD1	1:D:119:ASP:N	2.54	0.40
1:A:388:LYS:HB2	1:A:388:LYS:HE3	1.85	0.40
1:B:74:TYR:CD1	1:B:78:LYS:HD2	2.56	0.40
1:A:317:ARG:CZ	2:R:32:A:OP2	2.69	0.40
1:E:165:LYS:C	1:E:167:ILE:HD12	2.41	0.40
1:E:257:GLU:OE2	1:E:294:ASN:HA	2.21	0.40
1:A:8:ILE:HG13	1:A:9:ILE:N	2.37	0.40
1:A:182:PHE:CD1	1:A:182:PHE:C	2.94	0.40
1:B:342:ALA:HB3	1:B:344:LEU:HD23	2.03	0.40
1:C:344:LEU:CD2	1:C:344:LEU:N	2.83	0.40
1:A:202:PHE:CD2	1:A:211:ALA:HA	2.56	0.40
1:A:151:GLU:CD	2:R:33:A:H4'	2.42	0.40
1:C:138:LEU:HA	1:C:141:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:PHE:C	1:C:182:PHE:CD1	2.94	0.40
1:C:150:PRO:HA	1:C:152:TYR:CD1	2.52	0.40
1:A:74:TYR:CD1	1:A:78:LYS:HD2	2.57	0.40
1:B:382:PHE:O	1:B:385:GLN:N	2.45	0.40
1:A:104:ILE:CG2	1:A:104:ILE:O	2.68	0.40
1:D:218:ILE:C	1:D:220:SER:H	2.25	0.40
1:A:177:GLU:CA	1:A:181:ILE:HD11	2.35	0.40
1:C:99:GLY:O	1:C:100:ASP:C	2.60	0.40
1:D:44:THR:CA	1:D:46:LYS:CD	2.91	0.40
1:C:141:LEU:HD23	1:C:182:PHE:CZ	2.56	0.40
1:B:131:ASP:O	1:B:133:TRP:N	2.55	0.40
1:B:171:PHE:O	1:B:171:PHE:CD1	2.74	0.40
1:A:14:ILE:HD11	1:B:262:MET:HB2	2.03	0.40
1:E:91:PHE:CZ	1:E:267:GLU:HG3	2.57	0.40
1:D:181:ILE:HD12	1:D:183:ASP:OD2	2.22	0.40
1:D:171:PHE:CZ	1:D:173:PRO:O	2.74	0.40
1:B:153:ARG:CZ	1:B:176:PRO:C	2.90	0.40
1:E:128:SER:C	1:E:130:ASP:N	2.75	0.40
1:B:240:MET:HE3	1:B:240:MET:HB3	1.91	0.40
1:A:84:LEU:HA	1:A:84:LEU:HD23	1.88	0.40
1:C:4:THR:O	1:C:4:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	419/421 (100%)	306 (73%)	84 (20%)	29 (7%)	1 7
1	B	411/421 (98%)	305 (74%)	72 (18%)	34 (8%)	1 5
1	C	409/421 (97%)	301 (74%)	78 (19%)	30 (7%)	1 6
1	D	412/421 (98%)	305 (74%)	73 (18%)	34 (8%)	1 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	419/421 (100%)	303 (72%)	81 (19%)	35 (8%)	1 5
All	All	2070/2105 (98%)	1520 (73%)	388 (19%)	162 (8%)	1 6

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	79	ASP
1	A	117	LEU
1	A	150	PRO
1	A	172	GLU
1	A	342	ALA
1	B	22	GLU
1	B	100	ASP
1	B	117	LEU
1	B	150	PRO
1	B	172	GLU
1	B	342	ALA
1	C	22	GLU
1	C	79	ASP
1	C	117	LEU
1	C	150	PRO
1	C	170	GLN
1	C	172	GLU
1	C	271	ALA
1	C	342	ALA
1	D	22	GLU
1	D	117	LEU
1	D	167	ILE
1	D	172	GLU
1	D	271	ALA
1	D	314	ARG
1	E	22	GLU
1	E	117	LEU
1	E	150	PRO
1	E	168	ASN
1	E	170	GLN
1	E	172	GLU
1	E	342	ALA
1	E	360	SER
1	E	365	THR
1	A	84	LEU

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Mol	Chain	Res	Type
1	A	120	GLY
1	A	239	GLY
1	A	271	ALA
1	A	365	THR
1	B	30	ASP
1	B	79	ASP
1	B	84	LEU
1	B	120	GLY
1	B	169	GLU
1	B	239	GLY
1	B	271	ALA
1	B	314	ARG
1	C	30	ASP
1	C	84	LEU
1	C	120	GLY
1	C	239	GLY
1	C	314	ARG
1	D	8	ILE
1	D	30	ASP
1	D	44	THR
1	D	79	ASP
1	D	80	ILE
1	D	84	LEU
1	D	100	ASP
1	D	120	GLY
1	D	150	PRO
1	D	182	PHE
1	D	239	GLY
1	D	342	ALA
1	E	30	ASP
1	E	44	THR
1	E	79	ASP
1	E	84	LEU
1	E	120	GLY
1	E	239	GLY
1	E	271	ALA
1	E	314	ARG
1	E	363	GLY
1	A	30	ASP
1	A	176	PRO
1	A	182	PHE
1	A	314	ARG

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Mol	Chain	Res	Type
1	A	337	ALA
1	A	360	SER
1	A	364	LEU
1	B	98	ALA
1	B	132	LYS
1	B	168	ASN
1	B	176	PRO
1	B	182	PHE
1	C	176	PRO
1	C	182	PHE
1	C	337	ALA
1	D	99	GLY
1	D	168	ASN
1	D	176	PRO
1	E	176	PRO
1	E	182	PHE
1	E	366	THR
1	A	60	LYS
1	A	80	ILE
1	A	132	LYS
1	B	47	SER
1	B	80	ILE
1	B	90	SER
1	B	337	ALA
1	C	47	SER
1	C	80	ILE
1	C	132	LYS
1	D	43	ASN
1	D	47	SER
1	D	132	LYS
1	D	337	ALA
1	E	43	ASN
1	E	47	SER
1	E	80	ILE
1	E	337	ALA
1	A	23	ASP
1	A	177	GLU
1	A	350	VAL
1	B	23	ASP
1	B	45	THR
1	B	60	LYS
1	B	88	TRP

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Mol	Chain	Res	Type
1	B	391	PRO
1	C	23	ASP
1	C	43	ASN
1	C	45	THR
1	C	60	LYS
1	C	90	SER
1	C	177	GLU
1	D	23	ASP
1	D	45	THR
1	D	60	LYS
1	D	177	GLU
1	D	350	VAL
1	E	23	ASP
1	E	45	THR
1	E	60	LYS
1	E	88	TRP
1	E	132	LYS
1	E	177	GLU
1	E	350	VAL
1	A	46	LYS
1	A	88	TRP
1	B	177	GLU
1	E	90	SER
1	A	391	PRO
1	B	28	PRO
1	B	167	ILE
1	B	268	ILE
1	B	350	VAL
1	C	350	VAL
1	C	391	PRO
1	D	108	VAL
1	E	268	ILE
1	A	108	VAL
1	B	108	VAL
1	C	28	PRO
1	C	108	VAL
1	D	268	ILE
1	D	391	PRO
1	E	108	VAL
1	A	268	ILE
1	D	28	PRO
1	C	167	ILE

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%)	291 (80%)	71 (20%)	1 9
1	B	358/362 (99%)	291 (81%)	67 (19%)	2 10
1	C	356/362 (98%)	286 (80%)	70 (20%)	1 9
1	D	359/362 (99%)	293 (82%)	66 (18%)	2 10
1	E	362/362 (100%)	291 (80%)	71 (20%)	1 9
All	All	1797/1810 (99%)	1452 (81%)	345 (19%)	2 10

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	31	TYR
1	A	36	LYS
1	A	40	LEU
1	A	46	LYS
1	A	55	VAL
1	A	80	ILE
1	A	87	ASP
1	A	107	LEU
1	A	108	VAL
1	A	114	ASP
1	A	119	ASP
1	A	122	SER
1	A	134	LEU
1	A	136	LEU
1	A	149	MET
1	A	152	TYR
1	A	153	ARG
1	A	156	LEU
1	A	158	ASP
1	A	160	LEU
1	A	161	THR
1	A	162	ASN

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Mol	Chain	Res	Type
1	A	165	LYS
1	A	167	ILE
1	A	168	ASN
1	A	169	GLU
1	A	170	GLN
1	A	171	PHE
1	A	172	GLU
1	A	174	LEU
1	A	177	GLU
1	A	179	ARG
1	A	180	ASP
1	A	181	ILE
1	A	183	ASP
1	A	187	ASN
1	A	195	VAL
1	A	209	GLU
1	A	217	THR
1	A	228	LEU
1	A	230	THR
1	A	237	ILE
1	A	242	THR
1	A	243	GLU
1	A	252	ARG
1	A	253	GLU
1	A	268	ILE
1	A	272	ASP
1	A	287	SER
1	A	291	SER
1	A	292	VAL
1	A	307	LEU
1	A	308	LEU
1	A	309	ARG
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	364	LEU
1	A	366	THR

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Mol	Chain	Res	Type
1	A	367	ASN
1	A	375	VAL
1	A	384	ASP
1	A	398	LYS
1	A	410	LYS
1	A	414	LYS
1	B	25	VAL
1	B	31	TYR
1	B	36	LYS
1	B	40	LEU
1	B	44	THR
1	B	46	LYS
1	B	55	VAL
1	B	80	ILE
1	B	87	ASP
1	B	107	LEU
1	B	108	VAL
1	B	114	ASP
1	B	119	ASP
1	B	122	SER
1	B	134	LEU
1	B	136	LEU
1	B	149	MET
1	B	152	TYR
1	B	153	ARG
1	B	156	LEU
1	B	157	MET
1	B	158	ASP
1	B	160	LEU
1	B	161	THR
1	B	162	ASN
1	B	165	LYS
1	B	172	GLU
1	B	174	LEU
1	B	177	GLU
1	B	179	ARG
1	B	180	ASP
1	B	181	ILE
1	B	183	ASP
1	B	187	ASN
1	B	195	VAL
1	B	209	GLU

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Mol	Chain	Res	Type
1	B	217	THR
1	B	228	LEU
1	B	230	THR
1	B	237	ILE
1	B	242	THR
1	B	243	GLU
1	B	252	ARG
1	B	253	GLU
1	B	268	ILE
1	B	272	ASP
1	B	287	SER
1	B	291	SER
1	B	292	VAL
1	B	307	LEU
1	B	308	LEU
1	B	309	ARG
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	356	THR
1	B	358	ASP
1	B	366	THR
1	B	375	VAL
1	B	384	ASP
1	B	385	GLN
1	B	398	LYS
1	B	410	LYS
1	B	414	LYS
1	C	25	VAL
1	C	31	TYR
1	C	36	LYS
1	C	40	LEU
1	C	44	THR
1	C	46	LYS
1	C	55	VAL
1	C	80	ILE
1	C	87	ASP
1	C	107	LEU
1	C	108	VAL

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Mol	Chain	Res	Type
1	C	114	ASP
1	C	119	ASP
1	C	122	SER
1	C	134	LEU
1	C	136	LEU
1	C	149	MET
1	C	152	TYR
1	C	153	ARG
1	C	156	LEU
1	C	157	MET
1	C	158	ASP
1	C	160	LEU
1	C	161	THR
1	C	162	ASN
1	C	165	LYS
1	C	167	ILE
1	C	169	GLU
1	C	170	GLN
1	C	171	PHE
1	C	172	GLU
1	C	177	GLU
1	C	179	ARG
1	C	180	ASP
1	C	181	ILE
1	C	183	ASP
1	C	187	ASN
1	C	195	VAL
1	C	209	GLU
1	C	217	THR
1	C	228	LEU
1	C	230	THR
1	C	237	ILE
1	C	242	THR
1	C	243	GLU
1	C	252	ARG
1	C	253	GLU
1	C	268	ILE
1	C	272	ASP
1	C	287	SER
1	C	291	SER
1	C	292	VAL
1	C	307	LEU

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Mol	Chain	Res	Type
1	C	308	LEU
1	C	309	ARG
1	C	311	THR
1	C	317	ARG
1	C	325	THR
1	C	327	LEU
1	C	332	LEU
1	C	344	LEU
1	C	352	ASP
1	C	356	THR
1	C	366	THR
1	C	375	VAL
1	C	384	ASP
1	C	385	GLN
1	C	398	LYS
1	C	410	LYS
1	C	414	LYS
1	D	25	VAL
1	D	31	TYR
1	D	36	LYS
1	D	40	LEU
1	D	44	THR
1	D	46	LYS
1	D	55	VAL
1	D	80	ILE
1	D	87	ASP
1	D	100	ASP
1	D	107	LEU
1	D	108	VAL
1	D	114	ASP
1	D	119	ASP
1	D	122	SER
1	D	134	LEU
1	D	136	LEU
1	D	149	MET
1	D	152	TYR
1	D	153	ARG
1	D	156	LEU
1	D	157	MET
1	D	158	ASP
1	D	160	LEU
1	D	161	THR

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Mol	Chain	Res	Type
1	D	162	ASN
1	D	165	LYS
1	D	171	PHE
1	D	177	GLU
1	D	179	ARG
1	D	180	ASP
1	D	181	ILE
1	D	183	ASP
1	D	187	ASN
1	D	195	VAL
1	D	209	GLU
1	D	217	THR
1	D	228	LEU
1	D	230	THR
1	D	237	ILE
1	D	242	THR
1	D	243	GLU
1	D	252	ARG
1	D	253	GLU
1	D	268	ILE
1	D	272	ASP
1	D	287	SER
1	D	291	SER
1	D	292	VAL
1	D	307	LEU
1	D	308	LEU
1	D	309	ARG
1	D	311	THR
1	D	317	ARG
1	D	325	THR
1	D	327	LEU
1	D	332	LEU
1	D	343	ASP
1	D	352	ASP
1	D	356	THR
1	D	358	ASP
1	D	375	VAL
1	D	384	ASP
1	D	398	LYS
1	D	410	LYS
1	D	414	LYS
1	E	25	VAL

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Mol	Chain	Res	Type
1	E	31	TYR
1	E	36	LYS
1	E	40	LEU
1	E	44	THR
1	E	46	LYS
1	E	55	VAL
1	E	80	ILE
1	E	87	ASP
1	E	107	LEU
1	E	108	VAL
1	E	114	ASP
1	E	119	ASP
1	E	122	SER
1	E	134	LEU
1	E	136	LEU
1	E	149	MET
1	E	152	TYR
1	E	153	ARG
1	E	156	LEU
1	E	157	MET
1	E	158	ASP
1	E	160	LEU
1	E	161	THR
1	E	162	ASN
1	E	165	LYS
1	E	168	ASN
1	E	171	PHE
1	E	172	GLU
1	E	177	GLU
1	E	179	ARG
1	E	180	ASP
1	E	181	ILE
1	E	183	ASP
1	E	187	ASN
1	E	195	VAL
1	E	209	GLU
1	E	217	THR
1	E	228	LEU
1	E	230	THR
1	E	237	ILE
1	E	242	THR
1	E	243	GLU

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Mol	Chain	Res	Type
1	E	252	ARG
1	E	253	GLU
1	E	268	ILE
1	E	272	ASP
1	E	287	SER
1	E	291	SER
1	E	292	VAL
1	E	307	LEU
1	E	308	LEU
1	E	309	ARG
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	356	THR
1	E	359	ASP
1	E	360	SER
1	E	361	THR
1	E	365	THR
1	E	366	THR
1	E	375	VAL
1	E	384	ASP
1	E	385	GLN
1	E	398	LYS
1	E	410	LYS
1	E	414	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	63	ASN
1	A	68	HIS
1	A	70	ASN
1	A	170	GLN
1	A	190	ASN
1	A	266	GLN
1	A	347	GLN
1	A	386	ASN
1	A	395	GLN

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Mol	Chain	Res	Type
1	B	63	ASN
1	B	68	HIS
1	B	70	ASN
1	B	190	ASN
1	B	266	GLN
1	B	347	GLN
1	B	395	GLN
1	C	11	ASN
1	C	68	HIS
1	C	70	ASN
1	C	190	ASN
1	C	266	GLN
1	C	347	GLN
1	C	386	ASN
1	C	395	GLN
1	D	63	ASN
1	D	68	HIS
1	D	70	ASN
1	D	190	ASN
1	D	266	GLN
1	D	347	GLN
1	D	386	ASN
1	D	395	GLN
1	E	11	ASN
1	E	68	HIS
1	E	70	ASN
1	E	170	GLN
1	E	190	ASN
1	E	266	GLN
1	E	347	GLN
1	E	386	ASN
1	E	395	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	44/45 (97%)	25 (56%)	3 (6%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	3	A
2	R	4	A
2	R	5	A
2	R	7	A
2	R	8	A
2	R	10	A
2	R	11	A
2	R	12	A
2	R	14	A
2	R	21	A
2	R	22	A
2	R	23	A
2	R	24	A
2	R	25	A
2	R	26	A
2	R	27	A
2	R	28	A
2	R	30	A
2	R	31	A
2	R	32	A
2	R	33	A
2	R	40	A
2	R	42	A
2	R	44	A
2	R	45	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	4	A
2	R	10	A
2	R	26	A

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 carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	421/421 (100%)	0.16	23 (5%) 29 11	64, 111, 191, 233	0
1	B	415/421 (98%)	-0.02	15 (3%) 46 20	63, 109, 178, 233	0
1	C	413/421 (98%)	0.09	14 (3%) 49 21	65, 109, 179, 233	0
1	D	416/421 (98%)	0.12	23 (5%) 29 11	64, 110, 180, 235	0
1	E	421/421 (100%)	0.11	19 (4%) 37 15	64, 111, 184, 240	0
2	R	45/45 (100%)	-0.24	0 100 100	109, 122, 145, 155	0
All	All	2131/2150 (99%)	0.08	94 (4%) 38 16	63, 111, 183, 240	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	SER	13.8
1	A	2	SER	12.8
1	E	2	SER	10.2
1	A	362	GLY	6.8
1	E	365	THR	6.5
1	C	357	PRO	6.4
1	E	363	GLY	6.2
1	D	2	SER	5.8
1	B	2	SER	5.6
1	D	98	ALA	5.6
1	D	366	THR	5.2
1	A	360	SER	5.2
1	A	363	GLY	5.1
1	E	362	GLY	4.7
1	D	171	PHE	4.5
1	E	114	ASP	4.5
1	A	365	THR	4.2
1	D	94	ASN	4.1
1	E	95	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	355	TYR	3.9
1	E	366	THR	3.8
1	D	367	ASN	3.8
1	D	158	ASP	3.7
1	A	361	THR	3.6
1	A	357	PRO	3.6
1	D	166	MET	3.4
1	D	172	GLU	3.4
1	B	93	ILE	3.3
1	B	122	SER	3.3
1	A	57	GLN	3.3
1	A	364	LEU	3.3
1	A	158	ASP	3.1
1	C	62	GLY	3.1
1	B	422	LYS	3.1
1	C	158	ASP	3.0
1	A	359	ASP	2.9
1	A	176	PRO	2.9
1	B	158	ASP	2.8
1	B	131	ASP	2.8
1	A	172	GLU	2.8
1	E	178	GLY	2.8
1	D	274	TYR	2.8
1	A	62	GLY	2.7
1	B	274	TYR	2.7
1	A	43	ASN	2.6
1	D	62	GLY	2.6
1	A	166	MET	2.6
1	A	83	LYS	2.5
1	E	364	LEU	2.5
1	C	83	LYS	2.5
1	E	83	LYS	2.5
1	C	59	LEU	2.5
1	D	355	TYR	2.5
1	A	98	ALA	2.5
1	C	114	ASP	2.4
1	B	172	GLU	2.4
1	D	43	ASN	2.4
1	D	56	TYR	2.4
1	D	57	GLN	2.4
1	E	96	GLY	2.4
1	B	365	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	92	GLY	2.4
1	C	366	THR	2.4
1	A	59	LEU	2.3
1	B	346	GLN	2.3
1	A	122	SER	2.3
1	D	60	LYS	2.3
1	D	121	VAL	2.3
1	E	172	GLU	2.3
1	D	365	THR	2.3
1	B	145	GLY	2.3
1	C	353	ASN	2.3
1	E	101	THR	2.3
1	A	111	LYS	2.3
1	C	122	SER	2.3
1	C	121	VAL	2.2
1	B	355	TYR	2.2
1	D	346	GLN	2.2
1	E	117	LEU	2.2
1	E	274	TYR	2.2
1	A	366	THR	2.2
1	D	112	ALA	2.1
1	C	178	GLY	2.1
1	D	122	SER	2.1
1	D	97	LYS	2.1
1	E	102	ILE	2.1
1	E	62	GLY	2.1
1	E	98	ALA	2.1
1	E	346	GLN	2.1
1	B	173	PRO	2.1
1	D	87	ASP	2.0
1	A	94	ASN	2.0
1	B	366	THR	2.0
1	C	98	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
3	IUM	A	522	1/3	1.00	0.16	-0.62	139,139,139,139	1
3	IUM	D	532	1/3	0.99	0.16	-0.64	136,136,136,136	1
3	IUM	C	529	1/3	0.99	0.15	-0.79	121,121,121,121	1
3	IUM	E	534	1/3	0.98	0.11	-1.68	152,152,152,152	0
3	IUM	C	528	1/3	0.97	0.12	-	131,131,131,131	1
3	IUM	R	540	1/3	0.99	0.12	-	157,157,157,157	1
3	IUM	E	533	1/3	0.97	0.15	-	144,144,144,144	1
3	IUM	R	537	1/3	0.98	0.14	-	132,132,132,132	1
3	IUM	R	536	1/3	0.97	0.14	-	156,156,156,156	1
3	IUM	D	531	1/3	0.94	0.14	-	134,134,134,134	1
3	IUM	B	525	1/3	0.98	0.14	-	143,143,143,143	1
3	IUM	A	521	1/3	0.94	0.13	-	145,145,145,145	1
3	IUM	R	538	1/3	0.99	0.14	-	128,128,128,128	1
3	IUM	C	530	1/3	0.96	0.09	-	199,199,199,199	0
3	IUM	A	524	1/3	0.97	0.10	-	197,197,197,197	1
3	IUM	B	526	1/3	1.00	0.14	-	152,152,152,152	0
3	IUM	R	539	1/3	0.96	0.14	-	153,153,153,153	1
3	IUM	E	535	1/3	0.96	0.15	-	175,175,175,175	1
3	IUM	A	523	1/3	0.98	0.11	-	193,193,193,193	1
3	IUM	B	527	1/3	0.95	0.10	-	163,163,163,163	1

6.5 Other polymers

There are no such residues in this entry.