Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 03:45 PM EST

PDB ID	:	3PU1
Title	:	Crystal Structure of a vesicular stomatitis virus nucleocapsid-polyG complex
Authors	:	Luo, M.; Green, T.J.; Rowse, M.
Deposited on	:	2010-12-03
Resolution	:	3.14 Å(reported)

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

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

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

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

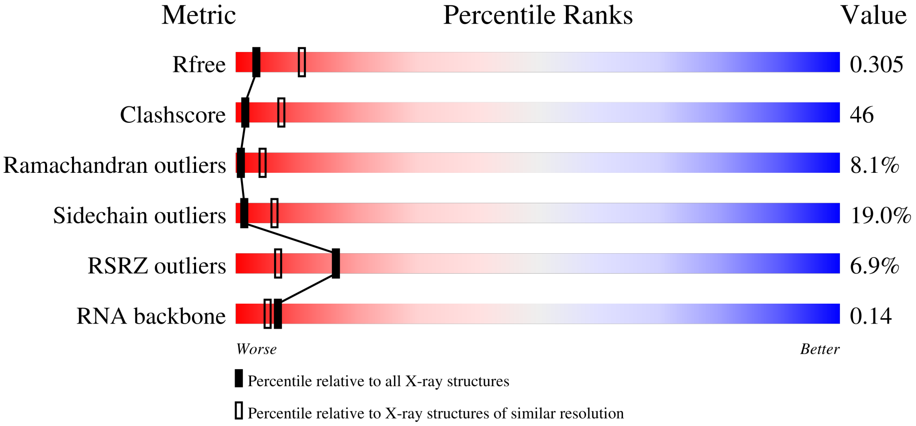
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

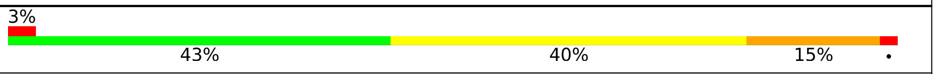
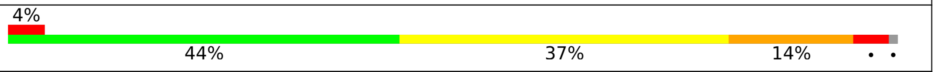
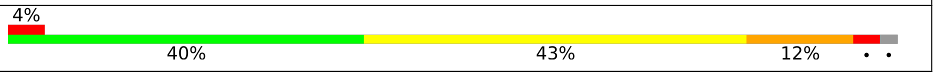
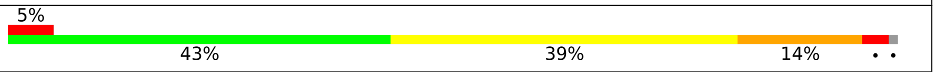
The reported resolution of this entry is 3.14 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)
RNA backbone	3102	1000 (3.46-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	
1	C	421	
1	D	421	

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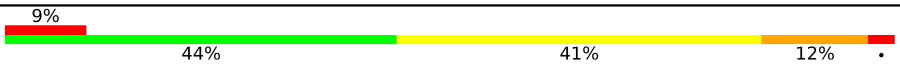
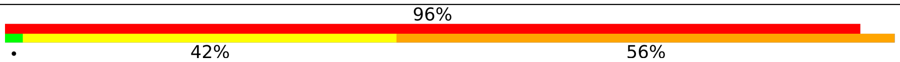
Mol	Chain	Length	Quality of chain
1	E	421	
2	R	45	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17572 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.

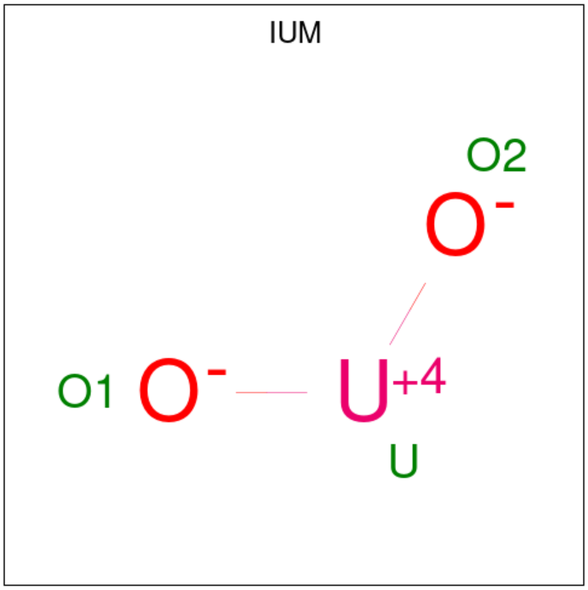
- Molecule 1 is a protein called Nucleoprotein.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	R	45	1035	450	225	315	45	0	0	0

- 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	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

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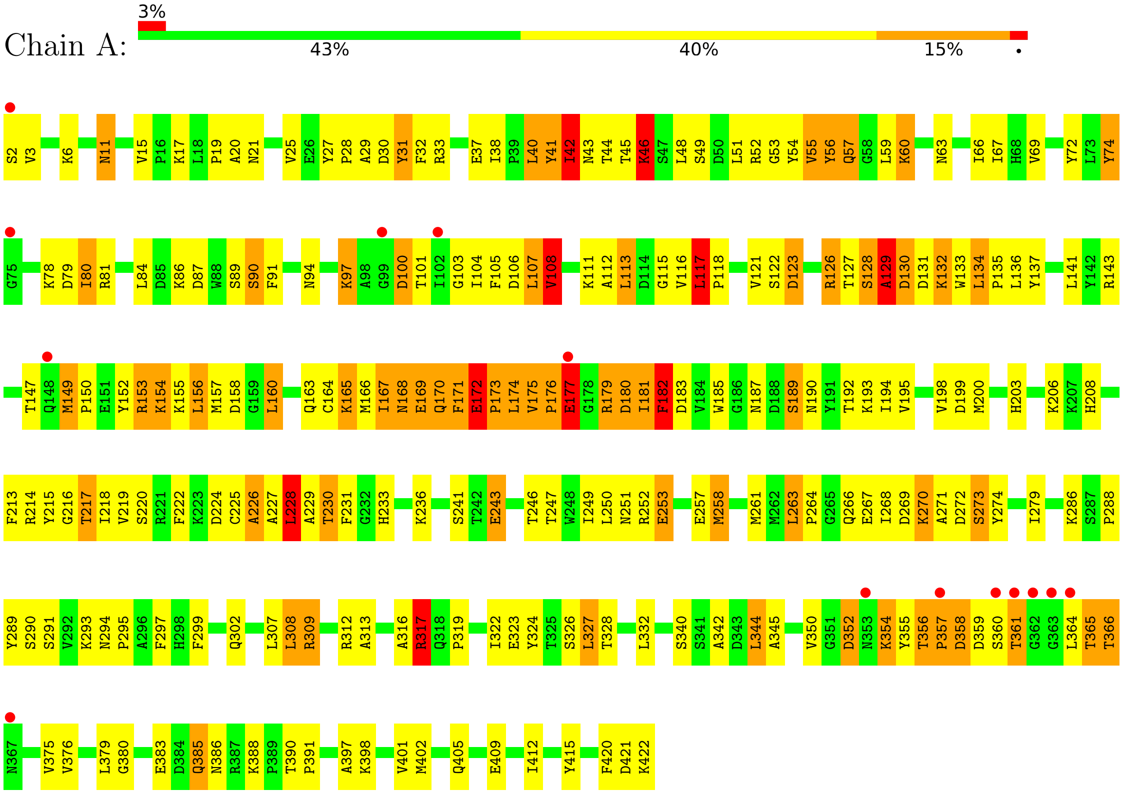
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0
3	R	1	Total U 1 1	0	0

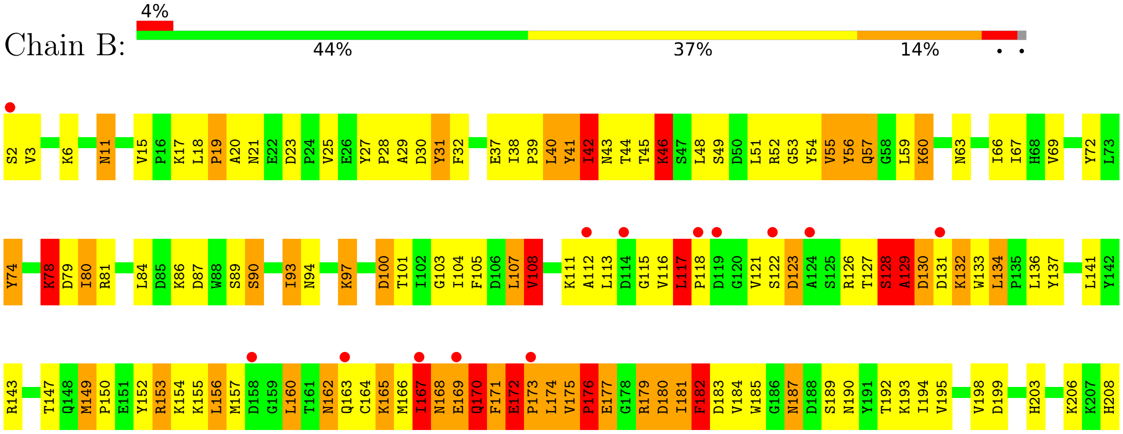
3 Residue-property plots ⓘ

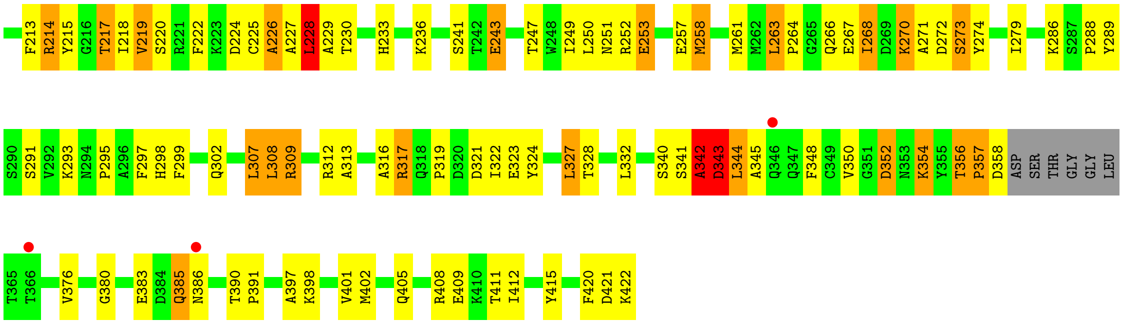
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Nucleoprotein

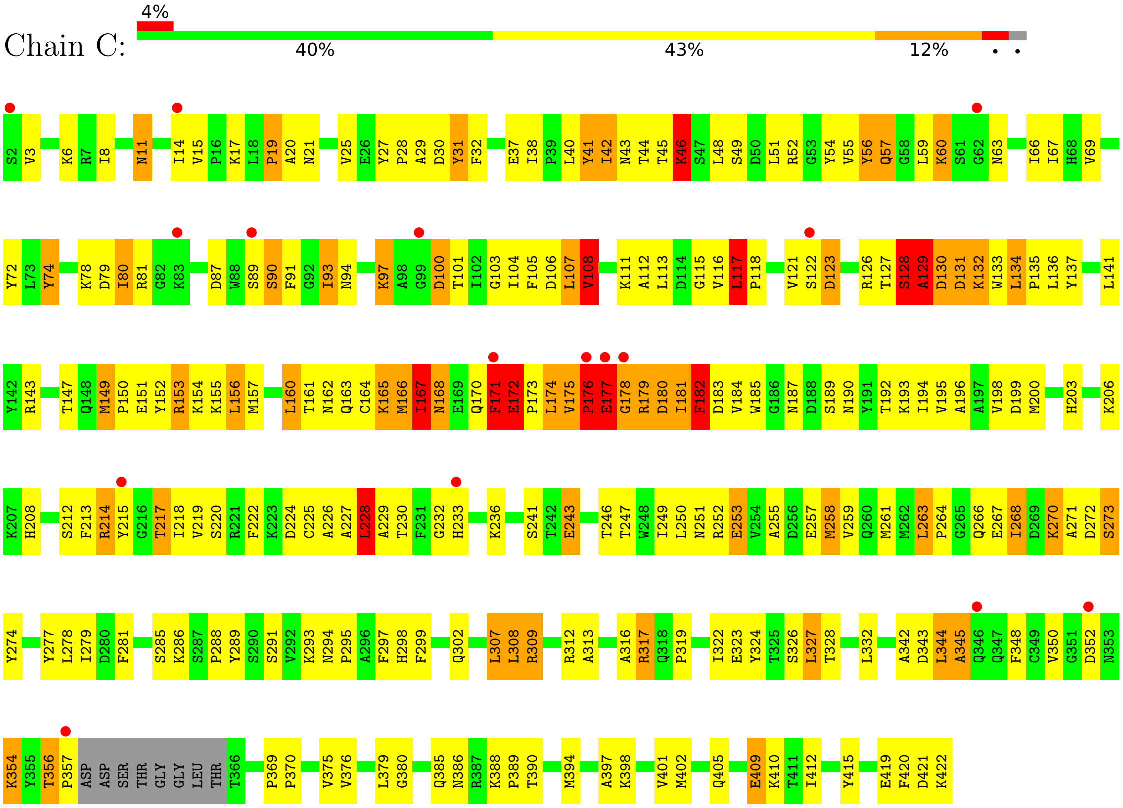


- Molecule 1: Nucleoprotein

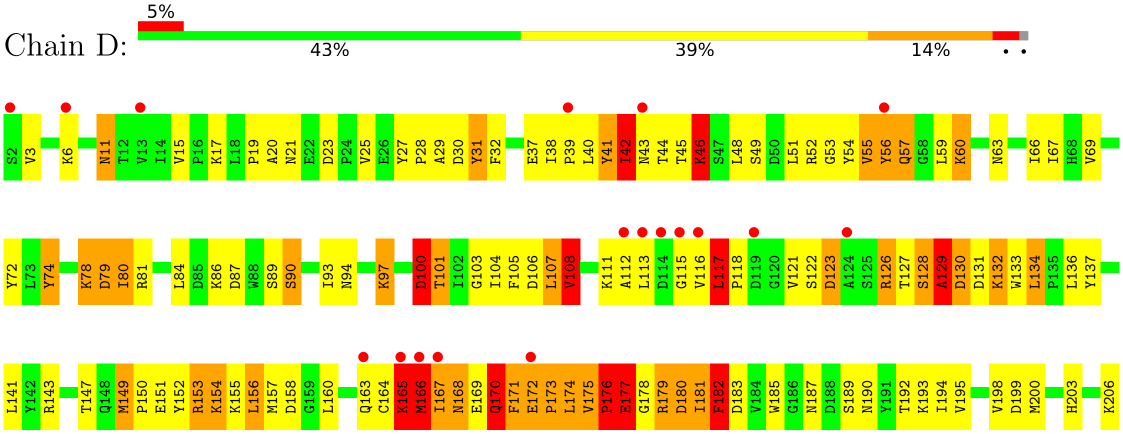


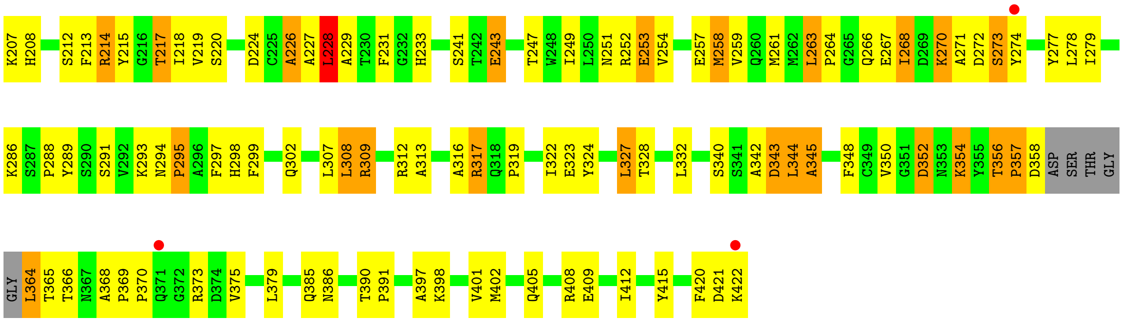


- Molecule 1: Nucleoprotein



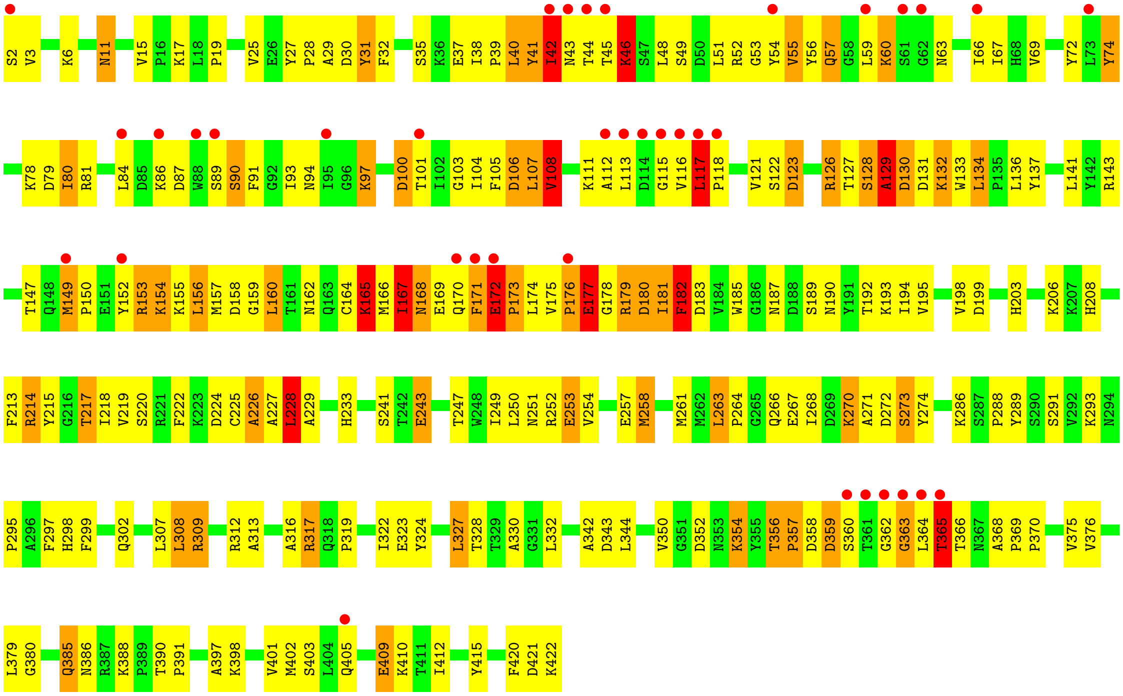
- Molecule 1: Nucleoprotein





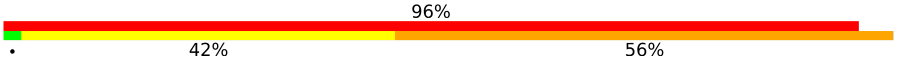
- Molecule 1: Nucleoprotein

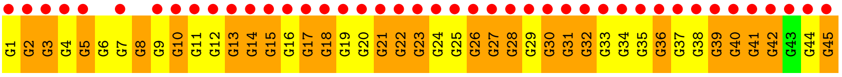
Chain E:



- Molecule 2: RNA (45-MER)

Chain R:





4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.22Å 233.19Å 75.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.10 – 3.14 45.14 – 3.14	Depositor EDS
% Data completeness (in resolution range)	79.0 (45.10-3.14) 79.0 (45.14-3.14)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.259 , 0.305 0.255 , 0.305	Depositor DCC
R_{free} test set	2000 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	76.3	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	17572	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/3403	0.75	6/4607 (0.1%)
1	B	0.50	0/3365	0.67	2/4554 (0.0%)
1	C	0.53	0/3350	0.76	8/4533 (0.2%)
1	D	0.50	0/3373	0.69	4/4565 (0.1%)
1	E	0.48	0/3403	0.71	6/4607 (0.1%)
2	R	0.93	0/1169	1.21	4/1841 (0.2%)
All	All	0.54	0/18063	0.76	30/24707 (0.1%)

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	5
1	B	0	8
1	C	0	4
1	D	0	6
1	E	0	7
All	All	0	30

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	GLU	N-CA-CB	-13.66	86.01	110.60
1	E	177	GLU	N-CA-CB	-13.58	86.15	110.60
1	C	171	PHE	CB-CA-C	-10.53	89.33	110.40
1	D	130	ASP	N-CA-CB	-9.40	93.68	110.60
1	C	130	ASP	N-CA-CB	-9.40	93.69	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	ASP	N-CA-CB	-9.33	93.80	110.60
1	E	130	ASP	N-CA-CB	-9.03	94.34	110.60
1	A	130	ASP	N-CA-CB	-8.81	94.73	110.60
1	C	172	GLU	N-CA-CB	-8.78	94.81	110.60
1	C	171	PHE	N-CA-C	8.46	133.85	111.00
1	A	345	ALA	N-CA-CB	-8.41	98.33	110.10
1	C	177	GLU	N-CA-CB	-8.02	96.17	110.60
1	C	172	GLU	N-CA-C	7.92	132.38	111.00
1	A	177	GLU	N-CA-C	7.59	131.50	111.00
1	E	177	GLU	N-CA-C	7.46	131.15	111.00
1	C	176	PRO	CB-CA-C	-7.38	93.56	112.00
1	A	176	PRO	CB-CA-C	-7.13	94.17	112.00
1	E	176	PRO	CB-CA-C	-6.75	95.14	112.00
2	R	15	G	C4-N9-C1’	6.57	135.04	126.50
1	D	177	GLU	N-CA-CB	-6.35	99.17	110.60
1	D	228	LEU	CA-CB-CG	6.35	129.90	115.30
1	B	228	LEU	CA-CB-CG	6.20	129.56	115.30
1	E	228	LEU	CA-CB-CG	6.07	129.25	115.30
1	C	228	LEU	CA-CB-CG	6.02	129.14	115.30
1	D	176	PRO	CB-CA-C	-5.99	97.04	112.00
1	A	228	LEU	CA-CB-CG	5.84	128.74	115.30
2	R	15	G	C8-N9-C1’	-5.69	119.60	127.00
2	R	15	G	N3-C4-N9	5.64	129.38	126.00
2	R	15	G	N3-C4-C5	-5.51	125.85	128.60
1	E	167	ILE	N-CA-C	5.05	124.63	111.00

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	LEU	Peptide
1	A	129	ALA	Peptide
1	A	169	GLU	Peptide
1	A	317	ARG	Sidechain
1	A	41	TYR	Peptide
1	B	107	LEU	Peptide
1	B	129	ALA	Peptide
1	B	176	PRO	Peptide
1	B	342	ALA	Peptide
1	B	343	ASP	Peptide
1	B	344	LEU	Peptide
1	B	41	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	B	78	LYS	Peptide
1	C	107	LEU	Peptide
1	C	129	ALA	Peptide
1	C	176	PRO	Peptide
1	C	41	TYR	Peptide
1	D	107	LEU	Peptide
1	D	129	ALA	Peptide
1	D	170	GLN	Peptide
1	D	176	PRO	Peptide
1	D	41	TYR	Peptide
1	D	78	LYS	Peptide
1	E	107	LEU	Peptide
1	E	129	ALA	Peptide
1	E	165	LYS	Peptide
1	E	169	GLU	Peptide
1	E	172	GLU	Peptide
1	E	363	GLY	Peptide
1	E	41	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3327	0	3287	332	0
1	B	3290	0	3253	345	0
1	C	3275	0	3242	326	0
1	D	3298	0	3264	321	0
1	E	3327	0	3287	292	0
2	R	1035	0	496	125	0
3	A	5	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	2	0	0	0	0
3	R	5	0	0	0	0
All	All	17572	0	16829	1572	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 46.

All (1572) 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:C:171:PHE:CG	1:C:171:PHE:O	1.78	1.31
1:C:171:PHE:O	1:C:171:PHE:CD2	1.91	1.23
1:A:326:SER:HB3	1:B:343:ASP:CB	1.72	1.19
1:D:166:MET:O	1:D:167:ILE:HG13	1.42	1.17
1:D:317:ARG:H	1:D:317:ARG:CZ	1.56	1.17
1:C:177:GLU:HA	1:C:181:ILE:HD11	1.20	1.16
1:D:212:SER:HA	2:R:9:G:C2	1.80	1.15
1:D:170:GLN:CG	1:D:171:PHE:HB3	1.75	1.15
1:A:326:SER:HB3	1:B:343:ASP:HB2	1.24	1.14
1:D:170:GLN:HG3	1:D:171:PHE:HB3	1.23	1.13
1:B:317:ARG:CZ	1:B:317:ARG:H	1.61	1.12
1:B:164:CYS:HA	1:B:168:ASN:HA	1.18	1.10
1:B:177:GLU:HA	1:B:181:ILE:HD11	1.28	1.09
1:E:59:LEU:HB3	1:E:172:GLU:HG2	1.33	1.09
1:A:317:ARG:CZ	1:A:317:ARG:H	1.65	1.08
1:D:177:GLU:HA	1:D:181:ILE:HD11	1.10	1.07
1:E:149:MET:HG3	2:R:42:G:O4’	1.55	1.06
1:E:317:ARG:CZ	1:E:317:ARG:H	1.67	1.05
1:C:143:ARG:HH22	2:R:17:G:H3’	1.18	1.04
1:C:317:ARG:CZ	1:C:317:ARG:H	1.71	1.04
1:E:43:ASN:HA	1:E:112:ALA:H	1.24	1.03
1:D:170:GLN:HG3	1:D:171:PHE:CB	1.89	1.03
1:D:43:ASN:HA	1:D:112:ALA:H	1.24	1.02
1:A:317:ARG:HH21	2:R:32:G:P	1.82	1.02
1:C:43:ASN:HA	1:C:112:ALA:H	1.21	1.02
1:C:181:ILE:H	1:C:181:ILE:HD12	1.25	0.99
1:A:166:MET:O	1:A:167:ILE:HG13	1.59	0.98
1:A:326:SER:CB	1:B:343:ASP:HB2	1.94	0.98
1:A:57:GLN:HE21	1:A:60:LYS:HZ2	0.98	0.98
1:A:43:ASN:HA	1:A:112:ALA:H	1.25	0.97
1:B:43:ASN:HA	1:B:112:ALA:H	1.28	0.97
1:B:187:ASN:CG	1:C:165:LYS:HE3	1.85	0.97
1:E:177:GLU:HA	1:E:181:ILE:HD11	1.44	0.96
1:E:57:GLN:HE21	1:E:60:LYS:HZ2	0.96	0.96
1:A:177:GLU:HA	1:A:181:ILE:HD11	1.45	0.96
1:B:42:ILE:HG13	1:B:74:TYR:HD2	1.30	0.95
1:D:165:LYS:O	1:D:166:MET:HB2	1.60	0.95
1:A:141:LEU:HD22	1:A:182:PHE:HE1	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ILE:HG13	1:C:74:TYR:HD2	1.27	0.95
1:A:42:ILE:HG13	1:A:74:TYR:HD2	1.29	0.94
1:C:57:GLN:HE21	1:C:60:LYS:HZ2	0.94	0.94
1:D:170:GLN:HG3	1:D:171:PHE:N	1.83	0.94
1:B:181:ILE:HD12	1:B:181:ILE:H	1.33	0.94
1:C:324:TYR:O	1:C:328:THR:HG23	1.68	0.94
1:E:37:GLU:HB2	1:E:108:VAL:HG11	1.46	0.94
1:C:141:LEU:HD22	1:C:182:PHE:HE1	1.32	0.93
1:E:133:TRP:CD1	1:E:167:ILE:HG12	2.04	0.93
1:C:37:GLU:HB2	1:C:108:VAL:HG11	1.52	0.92
1:D:149:MET:HG3	2:R:6:G:O4’	1.70	0.92
1:A:181:ILE:HD12	1:A:181:ILE:H	1.34	0.92
1:B:380:GLY:HA2	1:C:354:LYS:NZ	1.85	0.92
1:D:42:ILE:HG13	1:D:74:TYR:HD2	1.33	0.92
1:B:97:LYS:O	1:B:100:ASP:HB2	1.70	0.91
1:D:143:ARG:HH22	2:R:8:G:H3’	1.33	0.91
1:A:163:GLN:O	1:A:167:ILE:HB	1.70	0.91
1:E:42:ILE:HG13	1:E:74:TYR:HD2	1.33	0.90
1:B:176:PRO:O	1:B:181:ILE:HG12	1.72	0.90
1:D:177:GLU:CA	1:D:181:ILE:HD11	2.00	0.90
1:A:37:GLU:HB2	1:A:108:VAL:HG11	1.51	0.90
1:C:226:ALA:HB2	2:R:13:G:H5”	1.51	0.90
1:D:141:LEU:HD22	1:D:182:PHE:HE1	1.35	0.89
1:D:37:GLU:HB2	1:D:108:VAL:HG11	1.54	0.89
1:D:117:LEU:HB2	1:D:118:PRO:HD2	1.54	0.89
1:D:324:TYR:O	1:D:328:THR:HG23	1.72	0.89
1:B:37:GLU:HB2	1:B:108:VAL:HG11	1.52	0.89
1:C:143:ARG:HH22	2:R:17:G:C3’	1.85	0.89
1:E:141:LEU:HD22	1:E:182:PHE:HE1	1.36	0.89
1:D:177:GLU:HA	1:D:181:ILE:CD1	2.01	0.88
1:C:143:ARG:NH2	2:R:17:G:H3’	1.87	0.88
1:B:141:LEU:HD22	1:B:182:PHE:HE1	1.37	0.88
1:C:132:LYS:HB3	1:C:167:ILE:HD12	1.56	0.88
1:D:181:ILE:HD12	1:D:181:ILE:H	1.36	0.88
1:B:286:LYS:HD2	2:R:20:G:OP1	1.73	0.88
1:E:143:ARG:HH22	2:R:44:G:H3’	1.39	0.88
1:C:117:LEU:HB2	1:C:118:PRO:HD2	1.56	0.88
1:C:149:MET:HG3	2:R:15:G:O4’	1.74	0.87
1:B:57:GLN:HE21	1:B:60:LYS:HZ2	0.92	0.87
1:B:383:GLU:HG3	1:C:354:LYS:HE2	1.55	0.87
1:A:324:TYR:O	1:A:328:THR:HG23	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:LYS:O	1:D:100:ASP:HB2	1.74	0.87
1:A:165:LYS:O	1:A:167:ILE:HD12	1.74	0.87
1:B:57:GLN:HE21	1:B:60:LYS:NZ	1.71	0.87
1:B:117:LEU:HB2	1:B:118:PRO:HD2	1.56	0.87
1:C:214:ARG:HA	1:C:217:THR:HG22	1.54	0.87
1:E:214:ARG:HA	1:E:217:THR:HG22	1.56	0.86
1:E:117:LEU:HB2	1:E:118:PRO:HD2	1.57	0.86
1:A:97:LYS:O	1:A:100:ASP:HB2	1.76	0.85
1:B:133:TRP:CZ3	1:B:169:GLU:HG3	2.11	0.85
1:E:97:LYS:O	1:E:100:ASP:HB2	1.76	0.85
1:B:126:ARG:HH11	1:B:127:THR:H	1.24	0.85
1:A:126:ARG:HH11	1:A:127:THR:H	1.24	0.85
1:E:133:TRP:NE1	1:E:167:ILE:HG12	1.92	0.85
1:E:171:PHE:O	1:E:171:PHE:CD2	2.30	0.85
1:E:181:ILE:H	1:E:181:ILE:HD12	1.40	0.85
1:D:126:ARG:HH11	1:D:127:THR:H	1.22	0.84
1:C:97:LYS:O	1:C:100:ASP:HB2	1.77	0.84
1:C:57:GLN:HE21	1:C:60:LYS:NZ	1.76	0.84
1:A:326:SER:HB3	1:B:343:ASP:HB3	1.60	0.84
1:C:263:LEU:HD12	1:C:264:PRO:HD2	1.58	0.84
1:C:42:ILE:HG13	1:C:74:TYR:CD2	2.13	0.83
1:D:214:ARG:HA	1:D:217:THR:HG22	1.57	0.83
1:D:317:ARG:CZ	1:D:317:ARG:N	2.40	0.83
1:B:42:ILE:HG13	1:B:74:TYR:CD2	2.14	0.83
1:A:117:LEU:HB2	1:A:118:PRO:HD2	1.59	0.83
1:A:42:ILE:HG13	1:A:74:TYR:CD2	2.13	0.83
1:E:172:GLU:CB	1:E:173:PRO:HD3	2.07	0.83
1:D:170:GLN:HG3	1:D:171:PHE:CA	2.09	0.82
1:C:126:ARG:HH11	1:C:127:THR:H	1.27	0.82
1:B:324:TYR:O	1:B:328:THR:HG23	1.80	0.81
1:D:72:TYR:CE1	1:D:134:LEU:HD12	2.15	0.81
1:B:214:ARG:HA	1:B:217:THR:HG22	1.60	0.81
1:E:57:GLN:HE21	1:E:60:LYS:NZ	1.77	0.81
1:C:177:GLU:CA	1:C:181:ILE:HD11	2.07	0.81
1:E:126:ARG:HH11	1:E:127:THR:H	1.25	0.81
1:B:169:GLU:HA	1:B:169:GLU:OE1	1.78	0.81
1:A:57:GLN:HE21	1:A:60:LYS:NZ	1.79	0.81
1:A:326:SER:CB	1:B:343:ASP:CB	2.56	0.81
1:D:175:VAL:HG23	1:D:176:PRO:O	1.79	0.81
1:A:317:ARG:NH1	1:A:317:ARG:N	2.29	0.81
1:B:176:PRO:O	1:B:181:ILE:CG1	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:TYR:O	1:E:328:THR:HG23	1.82	0.80
1:A:214:ARG:HA	1:A:217:THR:HG22	1.62	0.80
1:B:72:TYR:CE1	1:B:134:LEU:HD12	2.17	0.80
1:C:177:GLU:HA	1:C:181:ILE:CD1	2.08	0.80
1:A:143:ARG:HH12	2:R:36:G:C5'	1.95	0.79
1:B:164:CYS:CA	1:B:168:ASN:HA	2.08	0.79
1:C:166:MET:C	1:C:167:ILE:HD13	2.01	0.79
1:C:175:VAL:HG23	1:C:176:PRO:O	1.82	0.79
1:D:42:ILE:HG13	1:D:74:TYR:CD2	2.18	0.78
1:C:72:TYR:CE1	1:C:134:LEU:HD12	2.17	0.78
1:A:317:ARG:H	1:A:317:ARG:NH1	1.80	0.78
1:C:356:THR:HG23	1:C:357:PRO:HD3	1.64	0.78
1:E:72:TYR:CE1	1:E:134:LEU:HD12	2.19	0.78
1:B:133:TRP:CE3	1:B:169:GLU:HG3	2.18	0.78
1:A:354:LYS:HE3	1:A:356:THR:HA	1.64	0.78
1:B:122:SER:O	1:B:123:ASP:HB3	1.83	0.78
1:C:312:ARG:HG3	2:R:14:G:C5	2.18	0.78
1:E:214:ARG:HA	1:E:217:THR:CG2	2.14	0.78
1:A:356:THR:HG23	1:A:357:PRO:HD3	1.65	0.78
1:E:354:LYS:HE3	1:E:356:THR:HA	1.64	0.78
1:A:365:THR:O	1:A:366:THR:HB	1.83	0.77
1:B:152:TYR:HE1	1:B:153:ARG:CZ	1.97	0.77
1:B:149:MET:HG3	2:R:24:G:O4'	1.84	0.77
1:A:72:TYR:CE1	1:A:134:LEU:HD12	2.20	0.77
1:D:179:ARG:HA	1:D:183:ASP:OD1	1.85	0.77
1:D:365:THR:HG23	1:D:366:THR:H	1.49	0.77
1:E:263:LEU:HD12	1:E:264:PRO:HD2	1.64	0.77
1:E:179:ARG:HA	1:E:183:ASP:OD1	1.85	0.77
1:B:354:LYS:HE3	1:B:356:THR:HA	1.65	0.77
1:C:214:ARG:HA	1:C:217:THR:CG2	2.15	0.77
1:D:152:TYR:HE1	1:D:153:ARG:CZ	1.97	0.77
1:D:166:MET:O	1:D:167:ILE:CG1	2.30	0.77
1:A:152:TYR:HE1	1:A:153:ARG:CZ	1.98	0.76
1:E:59:LEU:HB3	1:E:172:GLU:CG	2.12	0.76
1:A:317:ARG:CZ	1:A:317:ARG:N	2.47	0.76
1:E:122:SER:O	1:E:123:ASP:HB3	1.84	0.76
1:B:214:ARG:HA	1:B:217:THR:CG2	2.15	0.76
1:E:167:ILE:HG22	1:E:168:ASN:H	1.50	0.76
1:E:172:GLU:HB2	1:E:173:PRO:HD3	1.68	0.76
1:C:354:LYS:HE3	1:C:356:THR:HA	1.66	0.76
1:B:312:ARG:HG3	2:R:23:G:C4	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD12	1:C:232:GLY:CA	2.16	0.75
1:D:356:THR:HG23	1:D:357:PRO:HD3	1.68	0.75
1:B:250:LEU:HD13	1:C:344:LEU:HD12	1.66	0.75
1:E:42:ILE:HG13	1:E:74:TYR:CD2	2.19	0.75
1:D:175:VAL:CG2	1:D:176:PRO:O	2.35	0.75
1:B:356:THR:HG23	1:B:357:PRO:HD3	1.67	0.75
1:A:214:ARG:HA	1:A:217:THR:CG2	2.16	0.75
1:D:214:ARG:HA	1:D:217:THR:CG2	2.17	0.75
1:C:122:SER:O	1:C:123:ASP:HB3	1.85	0.74
1:D:354:LYS:HE3	1:D:356:THR:HA	1.67	0.74
2:R:19:G:H2’	2:R:20:G:H5’	1.67	0.74
1:A:122:SER:O	1:A:123:ASP:HB3	1.87	0.74
1:B:383:GLU:HG3	1:C:354:LYS:CE	2.15	0.74
1:D:122:SER:O	1:D:123:ASP:HB3	1.85	0.74
1:C:179:ARG:HA	1:C:183:ASP:OD1	1.88	0.74
1:E:152:TYR:HE1	1:E:153:ARG:CZ	2.01	0.74
1:C:152:TYR:HE1	1:C:153:ARG:CZ	2.00	0.74
1:C:250:LEU:HD13	1:D:344:LEU:HD12	1.68	0.74
1:C:376:VAL:HG13	1:D:354:LYS:HB2	1.68	0.74
1:D:263:LEU:HD12	1:D:264:PRO:HD2	1.68	0.74
1:E:167:ILE:HG22	1:E:168:ASN:N	2.03	0.74
1:D:343:ASP:OD2	1:D:373:ARG:NH2	2.21	0.74
1:E:288:PRO:HG2	1:E:289:TYR:CE2	2.24	0.73
1:D:74:TYR:CE1	1:D:78:LYS:HD2	2.24	0.73
1:C:56:TYR:HD1	1:C:126:ARG:HB2	1.54	0.73
1:A:263:LEU:HD12	1:A:264:PRO:HD2	1.70	0.73
1:B:141:LEU:HD12	1:B:185:TRP:CZ3	2.24	0.73
1:D:56:TYR:HD1	1:D:126:ARG:HB2	1.53	0.73
1:B:165:LYS:O	1:B:167:ILE:HD12	1.87	0.72
1:A:317:ARG:NH2	2:R:32:G:OP2	2.22	0.72
1:A:56:TYR:HD1	1:A:126:ARG:HB2	1.55	0.72
1:D:57:GLN:HE21	1:D:60:LYS:HZ3	1.36	0.72
1:E:56:TYR:HD1	1:E:126:ARG:HB2	1.54	0.72
1:B:133:TRP:CH2	1:B:169:GLU:HG3	2.24	0.72
1:D:57:GLN:HE21	1:D:60:LYS:NZ	1.87	0.72
1:A:165:LYS:HB2	1:A:165:LYS:NZ	2.05	0.72
1:B:179:ARG:HA	1:B:183:ASP:OD1	1.89	0.72
1:B:224:ASP:CG	2:R:21:G:H4’	2.10	0.72
1:C:263:LEU:HD12	1:C:264:PRO:CD	2.19	0.72
1:A:179:ARG:HA	1:A:183:ASP:OD1	1.89	0.72
1:C:141:LEU:HD13	1:C:182:PHE:HD1	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ARG:CZ	1:E:317:ARG:N	2.50	0.71
1:E:177:GLU:CA	1:E:181:ILE:HD11	2.20	0.71
1:B:166:MET:O	1:B:167:ILE:HG13	1.89	0.71
1:E:167:ILE:CG2	1:E:168:ASN:N	2.52	0.71
2:R:30:G:H2’	2:R:31:G:O4’	1.90	0.71
2:R:36:G:C2	2:R:37:G:H1’	2.25	0.71
1:E:117:LEU:CB	1:E:118:PRO:HD2	2.19	0.71
1:A:143:ARG:HH12	2:R:36:G:H5’	1.54	0.71
1:B:57:GLN:NE2	1:B:60:LYS:HZ2	1.77	0.71
1:D:117:LEU:CB	1:D:118:PRO:HD2	2.21	0.71
1:E:312:ARG:HG3	2:R:41:G:C2	2.26	0.71
1:A:344:LEU:N	1:A:344:LEU:CD2	2.52	0.71
1:B:263:LEU:HD12	1:B:264:PRO:HD2	1.72	0.71
1:B:317:ARG:CZ	1:B:317:ARG:N	2.46	0.71
1:A:344:LEU:HD11	1:E:330:ALA:HA	1.73	0.71
1:D:288:PRO:HG2	1:D:289:TYR:CE2	2.25	0.71
1:E:398:LYS:O	1:E:402:MET:HG2	1.91	0.71
1:D:224:ASP:CG	2:R:3:G:H4’	2.11	0.71
1:B:18:LEU:HD12	1:C:232:GLY:HA2	1.72	0.71
1:A:364:LEU:HD12	1:E:386:ASN:HD21	1.56	0.70
1:B:56:TYR:HD1	1:B:126:ARG:HB2	1.55	0.70
1:B:380:GLY:HA2	1:C:354:LYS:HZ3	1.56	0.70
1:E:356:THR:HG23	1:E:357:PRO:HD3	1.71	0.70
1:B:408:ARG:NH1	2:R:24:G:C8	2.59	0.70
1:A:299:PHE:CE1	1:A:328:THR:HG22	2.26	0.70
1:B:169:GLU:O	1:B:170:GLN:HB2	1.92	0.70
1:D:316:ALA:HA	1:D:317:ARG:NH2	2.06	0.70
1:C:250:LEU:HD13	1:D:344:LEU:CD1	2.20	0.70
1:C:298:HIS:NE2	1:C:317:ARG:NH1	2.39	0.70
1:D:308:LEU:O	1:D:309:ARG:HB2	1.90	0.70
1:A:316:ALA:HB1	1:A:317:ARG:HH12	1.57	0.70
1:A:359:ASP:C	1:A:361:THR:H	1.94	0.70
1:C:117:LEU:CB	1:C:118:PRO:HD2	2.22	0.70
1:A:105:PHE:C	1:A:107:LEU:H	1.94	0.70
1:B:308:LEU:O	1:B:309:ARG:HB2	1.91	0.70
1:B:165:LYS:HB2	1:B:165:LYS:NZ	2.07	0.69
1:B:79:ASP:HB2	1:B:81:ARG:HB2	1.72	0.69
1:B:288:PRO:HG2	1:B:289:TYR:CE2	2.27	0.69
1:B:133:TRP:CD2	1:B:169:GLU:CG	2.74	0.69
1:C:181:ILE:HD12	1:C:181:ILE:N	2.04	0.69
1:D:164:CYS:CB	1:D:168:ASN:HB3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD13	1:A:182:PHE:HD1	1.57	0.69
1:A:199:ASP:HB2	1:A:217:THR:HG23	1.74	0.69
1:C:233:HIS:HB2	1:C:312:ARG:NH1	2.07	0.69
1:B:141:LEU:HD13	1:B:182:PHE:HD1	1.56	0.69
1:B:167:ILE:O	1:B:168:ASN:O	2.10	0.69
1:A:117:LEU:CB	1:A:118:PRO:HD2	2.22	0.69
1:A:175:VAL:HG23	1:A:176:PRO:O	1.93	0.69
1:B:2:SER:HA	1:D:350:VAL:HG11	1.75	0.69
1:D:170:GLN:CG	1:D:171:PHE:N	2.55	0.69
1:E:59:LEU:CB	1:E:172:GLU:HG2	2.18	0.69
1:E:79:ASP:HB2	1:E:81:ARG:HB2	1.74	0.69
1:D:299:PHE:CE1	1:D:328:THR:HG22	2.27	0.69
1:A:74:TYR:CE1	1:A:78:LYS:HD2	2.27	0.69
1:B:133:TRP:CD2	1:B:169:GLU:HG2	2.28	0.69
1:A:288:PRO:HG2	1:A:289:TYR:CE2	2.28	0.68
1:C:179:ARG:HH22	2:R:11:G:N2	1.91	0.68
1:C:288:PRO:HG2	1:C:289:TYR:CE2	2.27	0.68
1:C:79:ASP:HB2	1:C:81:ARG:HB2	1.75	0.68
1:D:79:ASP:HB2	1:D:81:ARG:HB2	1.75	0.68
1:A:141:LEU:HD22	1:A:182:PHE:CE1	2.23	0.68
1:B:141:LEU:HB3	1:B:182:PHE:CE1	2.27	0.68
1:C:385:GLN:HG2	1:C:390:THR:HG22	1.75	0.68
1:E:167:ILE:O	1:E:168:ASN:HB2	1.93	0.68
1:A:117:LEU:HD23	1:A:117:LEU:N	2.09	0.68
1:B:143:ARG:HH22	2:R:26:G:H3’	1.57	0.68
1:D:170:GLN:CD	1:D:171:PHE:HB3	2.14	0.68
1:A:376:VAL:HG13	1:B:354:LYS:HB2	1.76	0.68
1:C:308:LEU:O	1:C:309:ARG:HB2	1.93	0.68
1:D:141:LEU:HD13	1:D:182:PHE:HD1	1.58	0.68
1:C:117:LEU:N	1:C:117:LEU:HD23	2.08	0.68
1:D:212:SER:HA	2:R:9:G:N1	2.09	0.68
1:A:224:ASP:CG	2:R:30:G:H4’	2.14	0.68
1:C:165:LYS:NZ	1:C:165:LYS:HB2	2.08	0.68
1:D:51:LEU:O	1:D:55:VAL:HG22	1.94	0.68
1:D:317:ARG:H	1:D:317:ARG:NH1	1.92	0.68
1:E:141:LEU:HD12	1:E:185:TRP:CZ3	2.29	0.68
1:E:263:LEU:HD12	1:E:264:PRO:CD	2.24	0.68
1:B:117:LEU:CB	1:B:118:PRO:HD2	2.23	0.67
1:B:350:VAL:HG11	1:E:2:SER:HA	1.76	0.67
1:B:181:ILE:H	1:B:181:ILE:CD1	2.02	0.67
1:D:398:LYS:O	1:D:402:MET:HG2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:H	1:A:181:ILE:CD1	2.03	0.67
1:E:317:ARG:HG3	2:R:40:G:C4	2.29	0.67
1:D:143:ARG:NH2	2:R:8:G:H3'	2.07	0.67
1:C:141:LEU:HD22	1:C:182:PHE:CE1	2.24	0.67
1:D:56:TYR:CD1	1:D:126:ARG:HB2	2.30	0.67
1:A:79:ASP:HB2	1:A:81:ARG:HB2	1.76	0.67
1:C:299:PHE:CE1	1:C:328:THR:HG22	2.29	0.67
1:E:141:LEU:HD13	1:E:182:PHE:HD1	1.59	0.67
1:B:132:LYS:HB3	1:B:167:ILE:HG12	1.77	0.67
1:C:57:GLN:NE2	1:C:60:LYS:HZ2	1.80	0.67
1:E:117:LEU:N	1:E:117:LEU:HD23	2.10	0.67
1:A:344:LEU:N	1:A:344:LEU:HD23	2.09	0.66
1:A:380:GLY:HA2	1:B:354:LYS:NZ	2.10	0.66
1:C:141:LEU:HD13	1:C:182:PHE:CD1	2.30	0.66
1:E:175:VAL:HG23	1:E:176:PRO:O	1.95	0.66
1:B:51:LEU:O	1:B:55:VAL:HG22	1.96	0.66
1:D:212:SER:HA	2:R:9:G:N2	2.10	0.66
1:C:66:ILE:HD12	1:C:69:VAL:HG21	1.78	0.66
1:C:344:LEU:O	1:C:345:ALA:HB2	1.95	0.66
1:A:250:LEU:HD13	1:B:344:LEU:HD12	1.77	0.66
1:C:326:SER:CB	1:D:343:ASP:OD1	2.44	0.66
1:C:56:TYR:CD1	1:C:126:ARG:HB2	2.30	0.66
1:D:44:THR:HG21	1:D:116:VAL:CG1	2.25	0.66
1:D:263:LEU:HD12	1:D:264:PRO:CD	2.25	0.66
1:B:133:TRP:CE3	1:B:169:GLU:CG	2.78	0.66
1:B:317:ARG:H	1:B:317:ARG:NH1	1.94	0.66
1:D:141:LEU:HD12	1:D:185:TRP:CZ3	2.31	0.66
2:R:16:G:H2'	2:R:17:G:H5'	1.76	0.66
1:E:105:PHE:C	1:E:107:LEU:H	2.00	0.66
1:A:166:MET:C	1:A:167:ILE:HG13	2.16	0.65
1:A:385:GLN:HG2	1:A:390:THR:HG22	1.76	0.65
1:B:105:PHE:C	1:B:107:LEU:H	2.00	0.65
1:E:74:TYR:CE1	1:E:78:LYS:HD2	2.31	0.65
1:A:141:LEU:HD12	1:A:185:TRP:CZ3	2.31	0.65
1:A:398:LYS:O	1:A:402:MET:HG2	1.95	0.65
1:B:298:HIS:NE2	1:B:317:ARG:NH1	2.44	0.65
1:E:308:LEU:O	1:E:309:ARG:HB2	1.95	0.65
1:B:385:GLN:HG2	1:B:390:THR:HG22	1.77	0.65
1:D:143:ARG:HE	1:D:155:LYS:HZ1	1.45	0.65
1:E:299:PHE:CE1	1:E:328:THR:HG22	2.32	0.65
1:C:74:TYR:CE1	1:C:78:LYS:HD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:PHE:C	1:C:107:LEU:H	1.98	0.65
1:D:129:ALA:HB1	1:D:167:ILE:HD13	1.79	0.65
1:D:141:LEU:HB3	1:D:182:PHE:CE1	2.30	0.65
1:E:298:HIS:NE2	1:E:317:ARG:NH1	2.43	0.65
1:A:56:TYR:CD1	1:A:126:ARG:HB2	2.31	0.65
1:B:383:GLU:HG3	1:C:354:LYS:NZ	2.12	0.65
2:R:34:G:H2’	2:R:35:G:O4’	1.96	0.65
1:A:385:GLN:HG2	1:A:390:THR:CG2	2.27	0.65
1:B:56:TYR:CD1	1:B:126:ARG:HB2	2.32	0.65
1:D:29:ALA:C	1:D:31:TYR:H	1.99	0.65
1:D:317:ARG:NH2	2:R:5:G:P	2.70	0.65
1:A:44:THR:HG21	1:A:116:VAL:CG1	2.27	0.65
1:C:141:LEU:HD12	1:C:185:TRP:CZ3	2.32	0.65
1:D:152:TYR:CE1	1:D:153:ARG:CZ	2.80	0.65
1:D:317:ARG:HH21	2:R:5:G:P	2.19	0.65
1:E:28:PRO:O	1:E:31:TYR:HB3	1.97	0.65
1:C:247:THR:HA	1:D:348:PHE:HB2	1.79	0.64
1:B:74:TYR:CE1	1:B:78:LYS:HD2	2.33	0.64
1:D:192:THR:HA	1:D:195:VAL:HG12	1.79	0.64
1:E:56:TYR:CD1	1:E:126:ARG:HB2	2.31	0.64
1:B:66:ILE:HD12	1:B:69:VAL:HG21	1.79	0.64
1:D:79:ASP:O	1:D:81:ARG:N	2.29	0.64
1:A:133:TRP:CG	1:A:167:ILE:HG21	2.33	0.64
1:A:177:GLU:CA	1:A:181:ILE:HD11	2.22	0.64
1:D:181:ILE:CD1	1:D:181:ILE:H	2.03	0.64
1:E:141:LEU:HB3	1:E:182:PHE:CE1	2.32	0.64
1:A:29:ALA:C	1:A:31:TYR:H	2.01	0.64
1:A:233:HIS:HB2	1:A:312:ARG:NH1	2.12	0.64
1:B:233:HIS:HB2	1:B:312:ARG:NH1	2.13	0.64
1:C:170:GLN:HG2	1:C:171:PHE:N	2.13	0.64
1:D:29:ALA:O	1:D:31:TYR:N	2.31	0.64
1:D:317:ARG:NH2	2:R:5:G:OP2	2.31	0.64
1:E:29:ALA:C	1:E:31:TYR:H	2.01	0.64
1:E:141:LEU:HD22	1:E:182:PHE:CE1	2.28	0.64
1:E:385:GLN:HG2	1:E:390:THR:HG22	1.79	0.64
1:A:263:LEU:HD12	1:A:264:PRO:CD	2.27	0.64
1:A:66:ILE:HD12	1:A:69:VAL:HG21	1.80	0.64
1:B:321:ASP:OD1	1:C:233:HIS:ND1	2.31	0.64
1:D:179:ARG:HG2	1:D:183:ASP:HB3	1.78	0.64
2:R:36:G:H2’	2:R:37:G:O4’	1.98	0.64
1:A:179:ARG:HG2	1:A:183:ASP:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TRP:HB3	1:B:167:ILE:HD13	1.80	0.64
1:E:179:ARG:HG2	1:E:183:ASP:HB3	1.80	0.64
1:C:55:VAL:HG23	1:C:56:TYR:H	1.63	0.63
1:A:165:LYS:HB2	1:A:165:LYS:HZ3	1.61	0.63
1:A:308:LEU:O	1:A:309:ARG:HB2	1.97	0.63
1:D:28:PRO:O	1:D:31:TYR:HB3	1.98	0.63
1:B:55:VAL:HG23	1:B:56:TYR:H	1.63	0.63
1:A:141:LEU:HB3	1:A:182:PHE:CE1	2.33	0.63
1:A:152:TYR:CE1	1:A:153:ARG:CZ	2.81	0.63
1:B:316:ALA:HA	1:B:317:ARG:NH2	2.14	0.63
1:B:152:TYR:CE1	1:B:153:ARG:CZ	2.80	0.63
1:D:141:LEU:HD22	1:D:182:PHE:CE1	2.26	0.63
1:E:364:LEU:O	1:E:365:THR:C	2.36	0.63
1:A:302:GLN:HE21	1:A:313:ALA:HB2	1.64	0.63
1:D:365:THR:HG23	1:D:366:THR:N	2.14	0.63
1:E:44:THR:HG21	1:E:116:VAL:CG1	2.27	0.63
1:E:171:PHE:CZ	1:E:173:PRO:O	2.51	0.63
1:A:344:LEU:HD23	1:A:344:LEU:H	1.64	0.63
1:B:44:THR:HG21	1:B:116:VAL:CG1	2.28	0.63
1:B:141:LEU:HD22	1:B:182:PHE:CE1	2.27	0.63
1:C:28:PRO:O	1:C:31:TYR:HB3	1.99	0.63
1:E:328:THR:HG21	1:E:415:TYR:OH	1.98	0.63
1:A:141:LEU:HD13	1:A:182:PHE:CD1	2.34	0.63
1:A:299:PHE:HE1	1:A:328:THR:HG22	1.62	0.63
1:B:192:THR:HA	1:B:195:VAL:HG12	1.81	0.63
2:R:16:G:C2'	2:R:17:G:H5'	2.28	0.63
1:B:179:ARG:HG2	1:B:183:ASP:HB3	1.81	0.63
1:B:299:PHE:CE1	1:B:328:THR:HG22	2.34	0.63
1:C:199:ASP:HB2	1:C:217:THR:HG23	1.81	0.63
2:R:37:G:C8	2:R:38:G:C8	2.88	0.62
1:D:199:ASP:HB2	1:D:217:THR:HG23	1.79	0.62
1:D:385:GLN:O	1:D:386:ASN:HB2	1.99	0.62
1:D:57:GLN:HA	1:D:60:LYS:HD3	1.81	0.62
1:D:105:PHE:C	1:D:107:LEU:H	2.01	0.62
1:C:263:LEU:CD1	1:C:264:PRO:HD2	2.27	0.62
1:D:117:LEU:CB	1:D:118:PRO:CD	2.78	0.62
1:E:342:ALA:HB1	1:E:344:LEU:HD23	1.80	0.62
1:A:175:VAL:CG2	1:A:176:PRO:O	2.48	0.62
1:B:117:LEU:CB	1:B:118:PRO:CD	2.77	0.62
1:B:250:LEU:HD13	1:C:344:LEU:CD1	2.30	0.62
1:C:117:LEU:CB	1:C:118:PRO:CD	2.77	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:HIS:NE2	1:D:317:ARG:NH1	2.47	0.62
1:A:385:GLN:O	1:A:386:ASN:HB2	1.98	0.62
1:C:184:VAL:HG13	1:D:165:LYS:HG3	1.81	0.62
1:D:117:LEU:HD23	1:D:117:LEU:N	2.14	0.62
1:B:263:LEU:HD12	1:B:264:PRO:CD	2.29	0.62
1:D:137:TYR:O	1:D:141:LEU:HG	2.00	0.62
1:D:385:GLN:HG2	1:D:390:THR:HG22	1.80	0.62
1:D:385:GLN:HG2	1:D:390:THR:CG2	2.30	0.62
1:A:137:TYR:O	1:A:141:LEU:HG	2.00	0.62
1:C:141:LEU:HB3	1:C:182:PHE:CE1	2.35	0.62
1:D:141:LEU:HD13	1:D:182:PHE:CD1	2.34	0.62
1:E:137:TYR:O	1:E:141:LEU:HG	1.99	0.62
1:B:317:ARG:O	1:B:319:PRO:HD3	2.00	0.62
1:C:44:THR:HG21	1:C:116:VAL:CG1	2.30	0.62
1:D:66:ILE:HD12	1:D:69:VAL:HG21	1.82	0.62
1:E:87:ASP:OD2	1:E:97:LYS:HG2	2.00	0.62
1:E:117:LEU:CB	1:E:118:PRO:CD	2.77	0.62
1:B:18:LEU:CD1	1:C:232:GLY:HA2	2.29	0.61
1:B:57:GLN:HA	1:B:60:LYS:HD3	1.82	0.61
1:C:179:ARG:HG2	1:C:183:ASP:HB3	1.81	0.61
1:E:316:ALA:HA	1:E:317:ARG:NH2	2.15	0.61
1:E:385:GLN:O	1:E:386:ASN:HB2	2.00	0.61
1:A:79:ASP:O	1:A:81:ARG:N	2.33	0.61
1:E:52:ARG:HD3	1:E:126:ARG:HG3	1.82	0.61
1:E:302:GLN:HE21	1:E:313:ALA:HB2	1.65	0.61
1:B:117:LEU:N	1:B:117:LEU:HD23	2.15	0.61
1:B:141:LEU:HD13	1:B:182:PHE:CD1	2.34	0.61
1:D:299:PHE:HE1	1:D:328:THR:HG22	1.65	0.61
1:D:343:ASP:OD2	1:D:373:ARG:CZ	2.48	0.61
1:E:66:ILE:HD12	1:E:69:VAL:HG21	1.81	0.61
1:E:141:LEU:HD13	1:E:182:PHE:CD1	2.35	0.61
1:E:199:ASP:HB2	1:E:217:THR:HG23	1.82	0.61
1:B:28:PRO:O	1:B:31:TYR:HB3	2.00	0.61
1:B:29:ALA:C	1:B:31:TYR:H	2.02	0.61
1:C:246:THR:HG22	1:D:348:PHE:CG	2.35	0.61
1:E:358:ASP:CG	1:E:359:ASP:H	2.04	0.61
1:C:192:THR:HA	1:C:195:VAL:HG12	1.82	0.61
1:E:175:VAL:CG2	1:E:176:PRO:O	2.48	0.61
1:A:192:THR:HA	1:A:195:VAL:HG12	1.82	0.61
1:A:199:ASP:CB	1:A:217:THR:HG23	2.30	0.61
1:E:316:ALA:HB1	1:E:317:ARG:HH12	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:ALA:CB	1:E:344:LEU:HD23	2.30	0.61
1:E:364:LEU:HB2	1:E:368:ALA:HB2	1.83	0.61
1:A:253:GLU:N	1:A:253:GLU:CD	2.54	0.61
1:C:66:ILE:HD12	1:C:69:VAL:CG2	2.31	0.61
1:C:87:ASP:OD2	1:C:97:LYS:HG2	2.01	0.61
1:C:107:LEU:HD23	1:C:274:TYR:CE2	2.36	0.61
1:A:51:LEU:O	1:A:55:VAL:HG22	2.01	0.61
1:A:55:VAL:HG23	1:A:56:TYR:H	1.66	0.61
1:A:57:GLN:NE2	1:A:60:LYS:HZ2	1.83	0.61
1:D:59:LEU:HD13	1:D:172:GLU:HG2	1.83	0.61
1:C:51:LEU:O	1:C:55:VAL:HG22	2.01	0.60
1:C:317:ARG:CZ	1:C:317:ARG:N	2.55	0.60
1:C:385:GLN:HG2	1:C:390:THR:CG2	2.31	0.60
2:R:20:G:H2’	2:R:21:G:O4’	2.01	0.60
1:A:365:THR:O	1:A:366:THR:CB	2.49	0.60
1:B:149:MET:HG3	2:R:24:G:C1’	2.32	0.60
1:D:126:ARG:HD3	1:D:127:THR:N	2.17	0.60
1:D:136:LEU:HD23	1:D:136:LEU:O	2.00	0.60
1:D:408:ARG:NH1	2:R:6:G:C8	2.69	0.60
1:E:354:LYS:CE	1:E:356:THR:HA	2.31	0.60
1:B:133:TRP:CD2	1:B:169:GLU:HG3	2.37	0.60
1:B:137:TYR:CE2	1:B:141:LEU:HD21	2.36	0.60
1:B:137:TYR:O	1:B:141:LEU:HG	2.01	0.60
1:B:398:LYS:O	1:B:402:MET:HG2	2.00	0.60
1:C:133:TRP:HB3	1:C:167:ILE:HG13	1.83	0.60
1:C:385:GLN:O	1:C:386:ASN:HB2	2.00	0.60
1:D:87:ASP:OD2	1:D:97:LYS:HG2	2.01	0.60
1:D:328:THR:HG21	1:D:415:TYR:OH	2.00	0.60
1:C:397:ALA:O	1:C:401:VAL:HG22	2.01	0.60
1:E:79:ASP:O	1:E:81:ARG:N	2.34	0.60
1:E:385:GLN:HG2	1:E:390:THR:CG2	2.30	0.60
2:R:32:G:H5”	2:R:33:G:OP1	2.01	0.60
1:E:317:ARG:HG3	2:R:40:G:C5	2.36	0.60
1:A:344:LEU:HD12	1:E:250:LEU:HD13	1.83	0.60
1:B:385:GLN:O	1:B:386:ASN:HB2	2.02	0.60
1:D:317:ARG:N	1:D:317:ARG:NH1	2.49	0.60
1:E:263:LEU:CD1	1:E:264:PRO:HD2	2.32	0.60
1:A:117:LEU:CB	1:A:118:PRO:CD	2.79	0.60
1:C:152:TYR:CE1	1:C:153:ARG:CZ	2.83	0.60
1:D:117:LEU:HB2	1:D:118:PRO:CD	2.31	0.60
1:E:57:GLN:HA	1:E:60:LYS:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:TYR:CE1	1:E:153:ARG:CZ	2.85	0.60
1:A:52:ARG:HD3	1:A:126:ARG:HG3	1.83	0.60
1:B:316:ALA:HB1	1:B:317:ARG:HH12	1.66	0.60
1:B:328:THR:HG21	1:B:415:TYR:OH	2.00	0.60
2:R:6:G:C8	2:R:6:G:O5'	2.55	0.60
1:D:59:LEU:HB3	1:D:172:GLU:HG3	1.84	0.60
1:E:51:LEU:O	1:E:55:VAL:HG22	2.01	0.60
1:E:227:ALA:HB1	1:E:261:MET:HE1	1.83	0.60
1:A:28:PRO:O	1:A:31:TYR:HB3	2.02	0.59
1:C:117:LEU:HB2	1:C:118:PRO:CD	2.31	0.59
1:C:212:SER:HB2	2:R:18:G:C6	2.36	0.59
1:C:246:THR:HG22	1:D:348:PHE:CD1	2.36	0.59
1:C:350:VAL:HG12	1:C:350:VAL:O	2.02	0.59
1:D:350:VAL:HG12	1:D:350:VAL:O	2.01	0.59
1:E:167:ILE:O	1:E:168:ASN:CB	2.50	0.59
1:C:57:GLN:HA	1:C:60:LYS:HD3	1.84	0.59
1:C:164:CYS:HA	1:C:168:ASN:HA	1.83	0.59
1:A:87:ASP:OD2	1:A:97:LYS:HG2	2.02	0.59
1:A:228:LEU:O	1:A:228:LEU:HD22	2.02	0.59
1:B:385:GLN:HG2	1:B:390:THR:CG2	2.31	0.59
1:C:143:ARG:HH22	2:R:17:G:C2'	2.15	0.59
1:D:263:LEU:CD1	1:D:264:PRO:HD2	2.32	0.59
1:E:365:THR:OG1	1:E:366:THR:N	2.33	0.59
2:R:17:G:O2'	2:R:18:G:P	2.59	0.59
1:A:107:LEU:HD23	1:A:274:TYR:CE2	2.37	0.59
1:A:133:TRP:HB3	1:A:167:ILE:HD13	1.84	0.59
1:B:181:ILE:HD12	1:B:181:ILE:N	2.13	0.59
1:B:187:ASN:ND2	1:C:165:LYS:HD3	2.18	0.59
1:C:29:ALA:C	1:C:31:TYR:H	2.04	0.59
1:B:302:GLN:HE21	1:B:313:ALA:HB2	1.67	0.59
1:D:55:VAL:HG23	1:D:56:TYR:H	1.67	0.59
1:D:253:GLU:N	1:D:253:GLU:CD	2.53	0.59
1:B:80:ILE:HA	1:B:103:GLY:HA3	1.85	0.59
1:C:354:LYS:CE	1:C:356:THR:HA	2.33	0.59
1:E:350:VAL:HG12	1:E:350:VAL:O	2.02	0.59
1:B:59:LEU:HB3	1:B:172:GLU:HG2	1.85	0.59
1:B:126:ARG:HD3	1:B:127:THR:N	2.18	0.59
1:A:66:ILE:HD13	1:A:185:TRP:CD1	2.38	0.59
1:B:153:ARG:HH12	1:B:176:PRO:HA	1.66	0.59
1:B:169:GLU:O	1:B:170:GLN:CB	2.51	0.59
1:B:267:GLU:HB3	1:B:270:LYS:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLN:HA	1:A:60:LYS:HD3	1.85	0.58
1:D:170:GLN:OE1	1:D:171:PHE:HB3	2.03	0.58
1:B:354:LYS:CE	1:B:356:THR:HA	2.33	0.58
1:C:52:ARG:HD3	1:C:126:ARG:HG3	1.84	0.58
1:D:317:ARG:CZ	2:R:5:G:OP2	2.51	0.58
1:C:317:ARG:O	1:C:319:PRO:HD3	2.03	0.58
1:D:354:LYS:CE	1:D:356:THR:HA	2.33	0.58
1:A:344:LEU:HD11	1:E:330:ALA:CA	2.34	0.58
1:D:66:ILE:HD13	1:D:185:TRP:CD1	2.39	0.58
1:A:227:ALA:C	1:A:229:ALA:H	2.07	0.58
1:C:14:ILE:HD12	1:D:259:VAL:HG22	1.86	0.58
1:D:286:LYS:HD2	2:R:2:G:OP1	2.04	0.58
1:C:153:ARG:HH12	1:C:176:PRO:HA	1.69	0.58
1:D:107:LEU:HD23	1:D:274:TYR:CE2	2.38	0.58
1:D:364:LEU:HD23	1:D:366:THR:N	2.19	0.58
1:D:153:ARG:HH12	1:D:176:PRO:HA	1.68	0.58
1:B:117:LEU:HB2	1:B:118:PRO:CD	2.31	0.58
1:C:171:PHE:O	1:C:171:PHE:CD1	2.53	0.58
1:D:126:ARG:HA	1:D:126:ARG:NH1	2.19	0.58
1:E:66:ILE:HD13	1:E:185:TRP:CD1	2.38	0.58
1:E:192:THR:HA	1:E:195:VAL:HG12	1.86	0.58
1:B:177:GLU:HA	1:B:181:ILE:CD1	2.19	0.58
1:B:341:SER:O	1:B:342:ALA:O	2.22	0.58
1:B:380:GLY:HA2	1:C:354:LYS:HZ2	1.67	0.58
1:D:151:GLU:HB2	2:R:6:G:O2’	2.04	0.58
1:E:171:PHE:CD2	1:E:171:PHE:C	2.77	0.58
1:B:194:ILE:O	1:B:198:VAL:HG23	2.04	0.57
1:B:227:ALA:O	1:B:229:ALA:N	2.37	0.57
1:B:253:GLU:N	1:B:253:GLU:CD	2.56	0.57
1:C:194:ILE:O	1:C:198:VAL:HG23	2.03	0.57
1:E:107:LEU:HD23	1:E:274:TYR:CE2	2.38	0.57
1:D:302:GLN:HE21	1:D:313:ALA:HB2	1.69	0.57
1:D:316:ALA:HB1	1:D:317:ARG:HH12	1.68	0.57
1:A:29:ALA:O	1:A:31:TYR:N	2.36	0.57
1:A:181:ILE:HD12	1:A:181:ILE:N	2.13	0.57
1:B:199:ASP:HB2	1:B:217:THR:HG23	1.87	0.57
1:C:137:TYR:O	1:C:141:LEU:HG	2.04	0.57
1:D:164:CYS:O	1:D:166:MET:N	2.31	0.57
1:D:344:LEU:O	1:D:345:ALA:HB2	2.03	0.57
1:A:317:ARG:O	1:A:319:PRO:HD3	2.03	0.57
1:C:175:VAL:CG2	1:C:176:PRO:O	2.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:GLN:HG3	1:D:60:LYS:HZ3	1.69	0.57
1:D:172:GLU:CB	1:D:173:PRO:HD3	2.34	0.57
1:E:29:ALA:O	1:E:31:TYR:N	2.35	0.57
1:E:253:GLU:CD	1:E:253:GLU:N	2.58	0.57
1:B:107:LEU:HD23	1:B:274:TYR:CE2	2.39	0.57
1:C:59:LEU:HB3	1:C:172:GLU:HG2	1.86	0.57
1:D:54:TYR:CD1	1:D:122:SER:HB3	2.39	0.57
1:A:397:ALA:O	1:A:401:VAL:HG22	2.05	0.57
1:C:165:LYS:HB2	1:C:165:LYS:HZ3	1.70	0.57
1:C:302:GLN:HE21	1:C:313:ALA:HB2	1.67	0.57
1:C:317:ARG:H	1:C:317:ARG:NH1	2.03	0.57
1:D:149:MET:HG3	2:R:6:G:C1’	2.34	0.57
1:D:227:ALA:C	1:D:229:ALA:H	2.07	0.57
1:E:164:CYS:O	1:E:165:LYS:C	2.40	0.57
1:A:143:ARG:NH2	2:R:35:G:C8	2.73	0.57
1:B:126:ARG:HD3	1:B:127:THR:H	1.69	0.57
1:C:288:PRO:HG2	1:C:289:TYR:CD2	2.40	0.57
1:C:421:ASP:O	1:C:422:LYS:HB3	2.04	0.57
1:E:181:ILE:H	1:E:181:ILE:CD1	2.05	0.57
1:A:59:LEU:HB3	1:A:172:GLU:HG2	1.87	0.57
1:B:52:ARG:HD3	1:B:126:ARG:HG3	1.86	0.57
1:B:153:ARG:O	1:B:157:MET:HG3	2.05	0.57
1:C:328:THR:HG21	1:C:415:TYR:OH	2.05	0.57
1:C:19:PRO:HA	1:D:268:ILE:O	2.04	0.57
1:C:199:ASP:CB	1:C:217:THR:HG23	2.34	0.57
1:C:299:PHE:HE1	1:C:328:THR:HG22	1.67	0.57
1:E:179:ARG:HA	1:E:183:ASP:CB	2.35	0.57
1:C:376:VAL:HG13	1:D:354:LYS:CB	2.35	0.57
1:D:267:GLU:HB3	1:D:270:LYS:HB2	1.87	0.57
1:C:137:TYR:CE2	1:C:141:LEU:HD21	2.39	0.56
1:C:326:SER:HB3	1:D:343:ASP:OD1	2.05	0.56
1:D:137:TYR:CE2	1:D:141:LEU:HD21	2.39	0.56
1:D:412:ILE:C	1:D:412:ILE:HD12	2.25	0.56
1:E:66:ILE:HD12	1:E:69:VAL:CG2	2.34	0.56
1:E:228:LEU:HD22	1:E:228:LEU:O	2.05	0.56
2:R:15:G:O5’	2:R:15:G:H8	1.88	0.56
1:A:182:PHE:N	1:A:182:PHE:HD2	2.03	0.56
1:D:199:ASP:CB	1:D:217:THR:HG23	2.35	0.56
1:A:143:ARG:HH12	2:R:36:G:H5”	1.68	0.56
1:A:194:ILE:O	1:A:198:VAL:HG23	2.06	0.56
1:A:267:GLU:HB3	1:A:270:LYS:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ARG:N	1:B:317:ARG:NH1	2.53	0.56
1:D:52:ARG:HD3	1:D:126:ARG:HG3	1.86	0.56
1:D:317:ARG:O	1:D:319:PRO:HD3	2.05	0.56
1:E:80:ILE:HA	1:E:103:GLY:HA3	1.87	0.56
1:A:380:GLY:HA2	1:B:354:LYS:HZ3	1.68	0.56
1:B:2:SER:O	1:C:243:GLU:HG3	2.05	0.56
1:D:164:CYS:HA	1:D:168:ASN:HB3	1.87	0.56
1:E:214:ARG:CA	1:E:217:THR:HG22	2.31	0.56
1:E:317:ARG:O	1:E:319:PRO:HD3	2.05	0.56
1:A:149:MET:HG3	2:R:33:G:C8	2.40	0.56
1:B:66:ILE:HD12	1:B:69:VAL:CG2	2.35	0.56
1:C:227:ALA:C	1:C:229:ALA:H	2.09	0.56
1:D:179:ARG:HA	1:D:183:ASP:CB	2.35	0.56
1:E:288:PRO:HG2	1:E:289:TYR:CD2	2.40	0.56
1:C:179:ARG:HA	1:C:183:ASP:CB	2.36	0.56
1:D:44:THR:HG21	1:D:116:VAL:HG13	1.86	0.56
1:B:79:ASP:O	1:B:81:ARG:N	2.38	0.56
1:E:41:TYR:HB2	1:E:190:ASN:HD21	1.70	0.56
1:B:166:MET:C	1:B:167:ILE:HG13	2.26	0.56
1:C:226:ALA:HB2	2:R:13:G:C5'	2.30	0.56
1:D:59:LEU:HB3	1:D:172:GLU:CG	2.36	0.56
1:D:153:ARG:O	1:D:157:MET:HG3	2.06	0.56
1:D:401:VAL:HG21	1:D:420:PHE:HB2	1.88	0.56
1:C:79:ASP:O	1:C:81:ARG:N	2.37	0.56
1:D:126:ARG:HD3	1:D:127:THR:H	1.70	0.56
1:E:199:ASP:CB	1:E:217:THR:HG23	2.34	0.56
1:C:66:ILE:HD13	1:C:185:TRP:CD1	2.42	0.55
1:C:151:GLU:HB2	2:R:15:G:O2'	2.06	0.55
1:D:74:TYR:CD1	1:D:78:LYS:HD2	2.41	0.55
1:A:388:LYS:HE2	1:B:340:SER:HB2	1.87	0.55
1:B:164:CYS:HA	1:B:168:ASN:CA	2.12	0.55
1:B:179:ARG:HA	1:B:183:ASP:CB	2.36	0.55
1:B:228:LEU:O	1:B:228:LEU:HD22	2.07	0.55
1:D:129:ALA:O	1:D:133:TRP:NE1	2.39	0.55
1:E:55:VAL:HG23	1:E:56:TYR:H	1.71	0.55
1:B:165:LYS:HB2	1:B:165:LYS:HZ3	1.71	0.55
1:A:137:TYR:CE2	1:A:141:LEU:HD21	2.42	0.55
1:A:179:ARG:HA	1:A:183:ASP:CB	2.37	0.55
1:C:143:ARG:HE	1:C:155:LYS:HZ1	1.54	0.55
1:C:170:GLN:HG2	1:C:171:PHE:HB3	1.89	0.55
1:C:228:LEU:HD22	1:C:228:LEU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:TYR:O	1:D:78:LYS:HD3	2.06	0.55
1:A:43:ASN:OD1	1:A:112:ALA:HB3	2.06	0.55
1:A:263:LEU:CD1	1:A:264:PRO:HD2	2.37	0.55
1:B:401:VAL:HG21	1:B:420:PHE:HB2	1.88	0.55
1:D:122:SER:O	1:D:123:ASP:CB	2.54	0.55
1:B:343:ASP:H	1:B:344:LEU:HD23	1.70	0.55
1:C:398:LYS:O	1:C:402:MET:HG2	2.05	0.55
1:D:286:LYS:HE2	1:D:293:LYS:HD3	1.87	0.55
1:D:295:PRO:HB2	1:D:322:ILE:CG2	2.37	0.55
1:A:317:ARG:NH2	2:R:32:G:OP1	2.40	0.55
1:B:44:THR:HG21	1:B:116:VAL:HG13	1.88	0.55
1:B:87:ASP:OD2	1:B:97:LYS:HG2	2.06	0.55
1:C:29:ALA:O	1:C:31:TYR:N	2.38	0.55
1:D:72:TYR:HE1	1:D:134:LEU:HB3	1.70	0.55
1:A:350:VAL:HG12	1:A:350:VAL:O	2.07	0.55
1:B:2:SER:HA	1:D:350:VAL:CG1	2.37	0.55
1:B:227:ALA:C	1:B:229:ALA:H	2.09	0.55
1:C:182:PHE:HD2	1:C:182:PHE:N	2.04	0.55
1:D:164:CYS:SG	1:D:168:ASN:HB3	2.47	0.55
1:D:166:MET:C	1:D:167:ILE:HG13	2.20	0.55
1:E:182:PHE:HD2	1:E:182:PHE:N	2.05	0.55
1:A:354:LYS:CE	1:A:356:THR:HA	2.34	0.55
1:C:182:PHE:N	1:C:182:PHE:CD2	2.75	0.55
1:E:117:LEU:HB2	1:E:118:PRO:CD	2.34	0.55
1:A:136:LEU:HD23	1:A:136:LEU:O	2.07	0.55
1:C:72:TYR:HE1	1:C:134:LEU:HB3	1.71	0.55
1:D:288:PRO:HG2	1:D:289:TYR:CD2	2.42	0.55
1:E:149:MET:HG3	2:R:42:G:C1’	2.36	0.55
1:E:227:ALA:C	1:E:229:ALA:H	2.09	0.55
1:B:136:LEU:HD23	1:B:136:LEU:O	2.05	0.54
1:E:171:PHE:CE1	1:E:173:PRO:O	2.60	0.54
1:E:267:GLU:HB3	1:E:270:LYS:HB2	1.89	0.54
1:A:66:ILE:HD12	1:A:69:VAL:CG2	2.37	0.54
1:A:117:LEU:HB2	1:A:118:PRO:CD	2.35	0.54
1:D:227:ALA:HB1	1:D:261:MET:HE1	1.89	0.54
1:A:286:LYS:HE2	1:A:293:LYS:HD3	1.88	0.54
1:B:182:PHE:HD2	1:B:182:PHE:N	2.05	0.54
1:E:43:ASN:HA	1:E:112:ALA:N	2.08	0.54
1:A:182:PHE:N	1:A:182:PHE:CD2	2.74	0.54
1:A:358:ASP:CG	1:A:359:ASP:H	2.01	0.54
1:B:126:ARG:NH1	1:B:127:THR:HG22	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:TYR:CE1	1:D:134:LEU:HB3	2.42	0.54
1:D:80:ILE:HA	1:D:103:GLY:HA3	1.89	0.54
1:D:170:GLN:CG	1:D:171:PHE:CB	2.61	0.54
1:A:317:ARG:NE	2:R:32:G:OP2	2.40	0.54
1:B:41:TYR:HB2	1:B:190:ASN:HD21	1.72	0.54
1:C:214:ARG:CA	1:C:217:THR:HG22	2.31	0.54
1:C:263:LEU:HD12	1:C:264:PRO:N	2.23	0.54
1:C:316:ALA:HB1	1:C:317:ARG:HH12	1.72	0.54
1:C:342:ALA:CB	1:C:344:LEU:HD23	2.38	0.54
1:E:299:PHE:HE1	1:E:328:THR:HG22	1.69	0.54
1:A:218:ILE:C	1:A:220:SER:H	2.11	0.54
1:C:253:GLU:CD	1:C:253:GLU:N	2.59	0.54
1:E:126:ARG:HA	1:E:126:ARG:NH1	2.22	0.54
1:E:412:ILE:C	1:E:412:ILE:HD12	2.28	0.54
1:B:179:ARG:O	1:C:161:THR:HG21	2.07	0.54
1:C:388:LYS:HE2	1:D:340:SER:HB2	1.89	0.54
1:C:401:VAL:HG21	1:C:420:PHE:HB2	1.90	0.54
1:E:137:TYR:CE2	1:E:141:LEU:HD21	2.43	0.54
1:D:228:LEU:O	1:D:228:LEU:HD22	2.08	0.54
1:B:54:TYR:CD1	1:B:122:SER:HB3	2.43	0.54
1:B:182:PHE:N	1:B:182:PHE:CD2	2.76	0.54
1:C:52:ARG:CD	1:C:126:ARG:HG3	2.38	0.54
1:D:74:TYR:O	1:D:74:TYR:HD1	1.91	0.54
1:E:44:THR:HG21	1:E:116:VAL:HG13	1.88	0.54
1:B:288:PRO:HG2	1:B:289:TYR:CD2	2.44	0.53
1:A:126:ARG:HD3	1:A:127:THR:N	2.24	0.53
1:A:250:LEU:HD13	1:B:344:LEU:CD1	2.38	0.53
1:B:74:TYR:O	1:B:78:LYS:HD3	2.09	0.53
1:B:227:ALA:HB1	1:B:261:MET:HE1	1.91	0.53
1:B:299:PHE:HE1	1:B:328:THR:HG22	1.73	0.53
1:C:192:THR:HA	1:C:195:VAL:CG1	2.39	0.53
1:E:52:ARG:CD	1:E:126:ARG:HG3	2.37	0.53
1:D:263:LEU:HD12	1:D:264:PRO:N	2.23	0.53
1:E:72:TYR:HE1	1:E:134:LEU:HB3	1.73	0.53
1:E:397:ALA:O	1:E:401:VAL:HG22	2.08	0.53
1:A:263:LEU:HD12	1:A:264:PRO:N	2.23	0.53
1:A:401:VAL:HG21	1:A:420:PHE:HB2	1.90	0.53
1:B:72:TYR:HE1	1:B:134:LEU:HB3	1.72	0.53
1:B:263:LEU:CD1	1:B:264:PRO:HD2	2.38	0.53
1:A:31:TYR:CD1	1:A:32:PHE:N	2.77	0.53
1:B:31:TYR:CD1	1:B:32:PHE:N	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ILE:HD13	1:B:185:TRP:CD1	2.44	0.53
1:B:263:LEU:HD12	1:B:264:PRO:N	2.23	0.53
1:B:356:THR:O	1:B:358:ASP:N	2.38	0.53
1:D:66:ILE:HD12	1:D:69:VAL:CG2	2.38	0.53
1:D:136:LEU:HB2	1:D:213:PHE:CE2	2.43	0.53
1:A:27:TYR:CZ	1:A:263:LEU:HD23	2.43	0.53
1:B:192:THR:HA	1:B:195:VAL:CG1	2.39	0.53
1:B:218:ILE:C	1:B:220:SER:H	2.11	0.53
1:A:44:THR:HG21	1:A:116:VAL:HG13	1.89	0.53
1:B:72:TYR:CE1	1:B:134:LEU:HB3	2.43	0.53
1:B:226:ALA:HB3	1:B:291:SER:HB3	1.91	0.53
1:C:326:SER:OG	1:D:343:ASP:OD1	2.26	0.53
2:R:19:G:C2’	2:R:20:G:H5’	2.37	0.53
1:A:317:ARG:H	1:A:317:ARG:NE	2.06	0.53
1:B:397:ALA:O	1:B:401:VAL:HG22	2.09	0.53
1:C:166:MET:O	1:C:167:ILE:HD13	2.08	0.53
1:D:227:ALA:O	1:D:229:ALA:N	2.40	0.53
1:E:317:ARG:N	1:E:317:ARG:NH1	2.57	0.53
1:E:317:ARG:H	1:E:317:ARG:NH1	2.03	0.53
1:A:126:ARG:NH1	1:A:126:ARG:HA	2.23	0.53
1:A:340:SER:HB2	1:E:388:LYS:HE2	1.91	0.53
1:A:421:ASP:O	1:A:422:LYS:HB3	2.07	0.53
1:B:129:ALA:O	1:B:133:TRP:NE1	2.42	0.53
1:C:31:TYR:CD1	1:C:32:PHE:N	2.77	0.53
1:C:179:ARG:HH22	2:R:11:G:H22	1.56	0.53
1:C:227:ALA:O	1:C:229:ALA:N	2.41	0.53
1:E:54:TYR:CD1	1:E:122:SER:HB3	2.44	0.53
1:A:169:GLU:HA	1:A:170:GLN:OE1	2.08	0.52
1:B:164:CYS:O	1:B:168:ASN:N	2.31	0.52
1:C:72:TYR:CE1	1:C:134:LEU:HB3	2.44	0.52
1:C:181:ILE:H	1:C:181:ILE:CD1	1.97	0.52
1:D:43:ASN:HA	1:D:112:ALA:N	2.09	0.52
2:R:17:G:O2’	2:R:18:G:O5’	2.24	0.52
1:A:177:GLU:HA	1:A:181:ILE:CD1	2.31	0.52
1:B:143:ARG:NH2	2:R:26:G:H2’	2.24	0.52
1:C:212:SER:CB	2:R:18:G:C6	2.92	0.52
1:C:316:ALA:HA	1:C:317:ARG:NH2	2.25	0.52
1:A:80:ILE:HA	1:A:103:GLY:HA3	1.91	0.52
1:A:133:TRP:HB3	1:A:167:ILE:CD1	2.39	0.52
1:B:162:ASN:N	1:B:162:ASN:HD22	2.07	0.52
1:B:199:ASP:CB	1:B:217:THR:HG23	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:TYR:CZ	1:C:263:LEU:HD23	2.45	0.52
1:C:126:ARG:NH1	1:C:127:THR:HG22	2.24	0.52
1:C:267:GLU:HB3	1:C:270:LYS:HB2	1.89	0.52
1:B:52:ARG:CD	1:B:126:ARG:HG3	2.40	0.52
1:B:421:ASP:O	1:B:422:LYS:HB3	2.09	0.52
1:D:215:TYR:C	1:D:215:TYR:CD2	2.83	0.52
1:D:317:ARG:H	1:D:317:ARG:NE	2.03	0.52
1:A:273:SER:OG	1:A:274:TYR:N	2.40	0.52
1:C:126:ARG:HD3	1:C:127:THR:N	2.24	0.52
1:C:177:GLU:HG2	1:C:181:ILE:HD11	1.92	0.52
1:E:74:TYR:CD1	1:E:78:LYS:HD2	2.45	0.52
1:E:143:ARG:NH2	2:R:44:G:H5”	2.25	0.52
1:C:72:TYR:HE1	1:C:134:LEU:HD12	1.73	0.52
1:C:89:SER:O	1:C:90:SER:HB2	2.09	0.52
1:C:155:LYS:HE3	2:R:17:G:OP2	2.09	0.52
1:D:214:ARG:CA	1:D:217:THR:HG22	2.34	0.52
1:E:129:ALA:HB1	1:E:167:ILE:HD11	1.91	0.52
1:B:143:ARG:HE	1:B:155:LYS:HZ1	1.57	0.52
1:C:129:ALA:HB1	1:C:133:TRP:HE1	1.75	0.52
1:C:136:LEU:O	1:C:136:LEU:HD23	2.09	0.52
1:D:189:SER:O	1:D:193:LYS:HG3	2.10	0.52
1:E:129:ALA:O	1:E:133:TRP:NE1	2.43	0.52
1:A:356:THR:O	1:A:358:ASP:N	2.38	0.52
1:B:143:ARG:HH22	2:R:26:G:C3’	2.23	0.52
1:B:162:ASN:HD22	1:B:162:ASN:H	1.56	0.52
1:B:224:ASP:OD1	2:R:21:G:H4’	2.10	0.52
1:B:228:LEU:O	1:B:228:LEU:HD13	2.10	0.52
1:C:43:ASN:OD1	1:C:112:ALA:HB3	2.10	0.52
1:E:31:TYR:CD1	1:E:32:PHE:N	2.77	0.52
1:B:29:ALA:O	1:B:31:TYR:N	2.36	0.52
1:C:44:THR:HG21	1:C:116:VAL:HG13	1.90	0.52
1:C:107:LEU:CD2	1:C:274:TYR:HE2	2.22	0.52
1:E:177:GLU:HA	1:E:181:ILE:CD1	2.30	0.52
1:E:356:THR:O	1:E:358:ASP:N	2.40	0.52
1:A:227:ALA:HB1	1:A:261:MET:HE1	1.91	0.52
1:A:328:THR:HG21	1:A:415:TYR:OH	2.10	0.52
1:B:133:TRP:CZ2	1:B:169:GLU:HG3	2.45	0.52
1:C:80:ILE:HA	1:C:103:GLY:HA3	1.93	0.52
1:E:136:LEU:O	1:E:136:LEU:HD23	2.10	0.52
1:A:189:SER:O	1:A:193:LYS:HG3	2.11	0.51
1:B:28:PRO:HD2	1:B:266:GLN:NE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:TYR:CD1	1:B:78:LYS:HD2	2.45	0.51
1:B:214:ARG:CA	1:B:217:THR:HG22	2.34	0.51
1:C:153:ARG:O	1:C:157:MET:HG3	2.10	0.51
1:B:350:VAL:HG12	1:B:350:VAL:O	2.11	0.51
1:C:129:ALA:O	1:C:133:TRP:NE1	2.43	0.51
1:E:126:ARG:NH1	1:E:127:THR:HG22	2.25	0.51
2:R:38:G:H2'	2:R:39:G:O4'	2.10	0.51
1:A:52:ARG:CD	1:A:126:ARG:HG3	2.40	0.51
1:A:107:LEU:CD2	1:A:274:TYR:HE2	2.22	0.51
1:A:227:ALA:O	1:A:229:ALA:N	2.43	0.51
1:B:152:TYR:CD1	1:B:177:GLU:HG3	2.44	0.51
1:C:41:TYR:HB2	1:C:190:ASN:HD21	1.75	0.51
1:D:168:ASN:OD1	1:D:168:ASN:N	2.43	0.51
1:E:107:LEU:CD2	1:E:274:TYR:HE2	2.24	0.51
1:E:267:GLU:OE1	1:E:273:SER:HB2	2.10	0.51
1:A:241:SER:OG	1:A:243:GLU:HG2	2.09	0.51
1:A:376:VAL:HG13	1:B:354:LYS:CB	2.39	0.51
1:B:45:THR:CB	1:B:111:LYS:HZ1	2.23	0.51
2:R:1:G:C2'	2:R:2:G:H5'	2.40	0.51
1:D:89:SER:O	1:D:90:SER:HB2	2.11	0.51
1:E:153:ARG:O	1:E:157:MET:HG3	2.10	0.51
1:A:126:ARG:NH1	1:A:127:THR:HG22	2.26	0.51
1:A:358:ASP:OD2	1:A:359:ASP:N	2.33	0.51
1:D:52:ARG:CD	1:D:126:ARG:HG3	2.40	0.51
1:E:6:LYS:NZ	1:E:11:ASN:HD21	2.09	0.51
1:E:263:LEU:HD12	1:E:264:PRO:N	2.26	0.51
1:E:317:ARG:H	1:E:317:ARG:NE	2.06	0.51
1:A:295:PRO:HB2	1:A:322:ILE:CG2	2.41	0.51
1:B:187:ASN:ND2	1:C:165:LYS:HE3	2.26	0.51
1:C:74:TYR:O	1:C:78:LYS:HD3	2.11	0.51
1:C:79:ASP:O	1:C:79:ASP:OD1	2.29	0.51
1:E:126:ARG:HD3	1:E:127:THR:N	2.25	0.51
1:E:291:SER:OG	2:R:40:G:H5"	2.11	0.51
1:A:43:ASN:HA	1:A:112:ALA:N	2.08	0.51
1:B:81:ARG:HD2	1:B:208:HIS:CE1	2.46	0.51
1:C:380:GLY:HA2	1:D:354:LYS:NZ	2.25	0.51
1:D:72:TYR:HE1	1:D:134:LEU:HD12	1.73	0.51
1:D:356:THR:O	1:D:358:ASP:N	2.38	0.51
1:E:72:TYR:CE1	1:E:134:LEU:HB3	2.45	0.51
2:R:10:G:C8	2:R:11:G:C8	2.99	0.51
1:B:104:ILE:HD13	1:B:198:VAL:HG22	1.93	0.51

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:B:415:TYR:HE2	1:C:309:ARG:HG2	1.76	0.51
1:C:226:ALA:HB3	1:C:291:SER:HB3	1.93	0.51
1:C:227:ALA:HB1	1:C:261:MET:HE1	1.92	0.51
1:E:172:GLU:N	1:E:173:PRO:CD	2.74	0.51
1:B:27:TYR:CZ	1:B:263:LEU:HD23	2.45	0.51
1:C:203:HIS:O	1:C:206:LYS:HG3	2.11	0.51
1:D:421:ASP:O	1:D:422:LYS:HB3	2.11	0.51
1:E:203:HIS:O	1:E:206:LYS:HG3	2.11	0.51
1:A:97:LYS:HB2	1:A:97:LYS:NZ	2.26	0.50
1:A:354:LYS:HB2	1:E:376:VAL:HG13	1.91	0.50
1:B:43:ASN:OD1	1:B:112:ALA:HB3	2.10	0.50
1:D:182:PHE:N	1:D:182:PHE:HD2	2.08	0.50
1:E:43:ASN:OD1	1:E:112:ALA:HB3	2.11	0.50
1:A:72:TYR:HE1	1:A:134:LEU:HB3	1.76	0.50
1:A:74:TYR:CD1	1:A:78:LYS:HD2	2.46	0.50
1:B:31:TYR:CD1	1:B:31:TYR:C	2.85	0.50
1:C:31:TYR:CD1	1:C:31:TYR:C	2.85	0.50
1:E:97:LYS:HB2	1:E:97:LYS:NZ	2.27	0.50
1:E:182:PHE:N	1:E:182:PHE:CD2	2.76	0.50
1:A:214:ARG:CA	1:A:217:THR:HG22	2.36	0.50
1:C:38:ILE:HD11	1:C:107:LEU:O	2.11	0.50
1:C:43:ASN:HA	1:C:112:ALA:N	2.07	0.50
1:C:74:TYR:CD1	1:C:74:TYR:C	2.85	0.50
1:A:288:PRO:HG2	1:A:289:TYR:CD2	2.46	0.50
1:D:107:LEU:CD2	1:D:274:TYR:HE2	2.24	0.50
1:D:181:ILE:HD12	1:D:181:ILE:N	2.16	0.50
1:E:129:ALA:HB1	1:E:133:TRP:HE1	1.76	0.50
1:D:27:TYR:CZ	1:D:263:LEU:HD23	2.47	0.50
1:D:81:ARG:HD2	1:D:208:HIS:CE1	2.47	0.50
1:E:31:TYR:CD1	1:E:31:TYR:C	2.84	0.50
1:A:129:ALA:HB1	1:A:133:TRP:HE1	1.76	0.50
1:B:2:SER:CA	1:D:350:VAL:HG11	2.42	0.50
1:C:45:THR:CB	1:C:111:LYS:HZ2	2.24	0.50
1:C:126:ARG:NH1	1:C:126:ARG:HA	2.26	0.50
2:R:19:G:H2'	2:R:20:G:C5'	2.38	0.50
1:A:74:TYR:O	1:A:78:LYS:HD3	2.12	0.50
1:D:203:HIS:O	1:D:206:LYS:HG3	2.12	0.50
1:E:74:TYR:O	1:E:78:LYS:HD3	2.11	0.50
2:R:6:G:C8	2:R:6:G:H3'	2.47	0.50
1:A:41:TYR:HB2	1:A:190:ASN:HD21	1.77	0.50
1:A:126:ARG:HD3	1:A:127:THR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:VAL:HG21	1:C:164:CYS:HB3	1.94	0.50
1:D:126:ARG:NH1	1:D:127:THR:HG22	2.27	0.50
1:D:182:PHE:N	1:D:182:PHE:CD2	2.79	0.50
1:E:194:ILE:O	1:E:198:VAL:HG23	2.12	0.50
1:E:286:LYS:HE2	1:E:293:LYS:HD3	1.93	0.50
1:A:122:SER:O	1:A:123:ASP:CB	2.59	0.50
1:A:152:TYR:CE1	1:A:177:GLU:HG3	2.47	0.50
1:B:136:LEU:HB2	1:B:213:PHE:CE2	2.47	0.50
1:C:74:TYR:C	1:C:74:TYR:HD1	2.15	0.50
1:C:286:LYS:HE2	1:C:293:LYS:HD3	1.94	0.50
1:D:41:TYR:HB2	1:D:190:ASN:HD21	1.77	0.50
1:D:43:ASN:OD1	1:D:112:ALA:HB3	2.11	0.50
1:D:192:THR:HA	1:D:195:VAL:CG1	2.40	0.50
1:C:126:ARG:HD3	1:C:127:THR:H	1.76	0.49
1:E:27:TYR:CZ	1:E:263:LEU:HD23	2.46	0.49
1:A:48:LEU:HD12	1:A:48:LEU:O	2.12	0.49
1:A:165:LYS:O	1:A:167:ILE:CD1	2.55	0.49
1:B:79:ASP:O	1:B:79:ASP:OD1	2.29	0.49
1:E:421:ASP:O	1:E:422:LYS:HB3	2.10	0.49
2:R:3:G:H2'	2:R:4:G:O4'	2.12	0.49
1:A:136:LEU:HB2	1:A:213:PHE:CE2	2.48	0.49
1:A:224:ASP:OD1	2:R:30:G:H4'	2.12	0.49
1:B:74:TYR:O	1:B:74:TYR:HD1	1.96	0.49
1:B:133:TRP:CE2	1:B:169:GLU:CG	2.95	0.49
1:C:107:LEU:HD23	1:C:274:TYR:HE2	1.78	0.49
1:D:253:GLU:CD	1:D:253:GLU:H	2.15	0.49
1:E:107:LEU:HD23	1:E:274:TYR:HE2	1.77	0.49
2:R:6:G:H3'	2:R:6:G:H8	1.76	0.49
1:A:105:PHE:C	1:A:107:LEU:N	2.64	0.49
1:A:153:ARG:O	1:A:157:MET:HG3	2.12	0.49
1:B:126:ARG:NH1	1:B:126:ARG:HA	2.28	0.49
1:D:56:TYR:CE1	1:D:126:ARG:NE	2.81	0.49
1:E:181:ILE:HD12	1:E:181:ILE:N	2.17	0.49
1:A:364:LEU:CD1	1:E:386:ASN:HD21	2.26	0.49
1:B:162:ASN:N	1:B:162:ASN:ND2	2.60	0.49
1:C:48:LEU:HD12	1:C:48:LEU:O	2.12	0.49
1:C:389:PRO:HG2	1:C:394:MET:HE1	1.95	0.49
1:D:74:TYR:CD1	1:D:74:TYR:C	2.86	0.49
1:D:79:ASP:HB2	1:D:81:ARG:NE	2.27	0.49
1:E:401:VAL:HG21	1:E:420:PHE:HB2	1.92	0.49
1:A:192:THR:HA	1:A:195:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PRO:HB2	1:B:322:ILE:CG2	2.42	0.49
1:C:170:GLN:NE2	1:C:171:PHE:HD2	2.11	0.49
1:E:81:ARG:HD2	1:E:208:HIS:CE1	2.47	0.49
1:A:31:TYR:CD1	1:A:31:TYR:C	2.86	0.49
1:A:81:ARG:HD2	1:A:208:HIS:CE1	2.48	0.49
1:A:249:ILE:CD1	1:A:258:MET:HG3	2.43	0.49
1:B:97:LYS:HB2	1:B:97:LYS:NZ	2.28	0.49
1:B:133:TRP:CE2	1:B:169:GLU:HG3	2.47	0.49
1:C:136:LEU:HB2	1:C:213:PHE:CE2	2.48	0.49
1:E:89:SER:O	1:E:90:SER:HB2	2.12	0.49
1:E:152:TYR:CE1	1:E:177:GLU:HG3	2.47	0.49
1:E:261:MET:HE3	1:E:297:PHE:CD2	2.48	0.49
1:B:46:LYS:HA	1:B:46:LYS:HD3	1.52	0.49
2:R:8:G:H5"	2:R:9:G:OP2	2.13	0.49
1:B:107:LEU:CD2	1:B:274:TYR:HE2	2.26	0.49
1:C:74:TYR:CD1	1:C:78:LYS:HD2	2.47	0.49
1:D:104:ILE:HD13	1:D:198:VAL:HG22	1.95	0.49
1:D:233:HIS:HB2	1:D:312:ARG:NH1	2.27	0.49
1:E:15:VAL:O	1:E:17:LYS:HG2	2.12	0.49
2:R:27:G:N3	2:R:27:G:O4'	2.45	0.49
1:C:117:LEU:N	1:C:117:LEU:CD2	2.74	0.49
1:A:45:THR:CB	1:A:111:LYS:HZ2	2.26	0.48
1:B:317:ARG:H	1:B:317:ARG:NE	2.05	0.48
1:C:74:TYR:O	1:C:74:TYR:HD1	1.96	0.48
1:C:342:ALA:HB1	1:C:344:LEU:HD23	1.95	0.48
1:C:380:GLY:HA2	1:D:354:LYS:HZ3	1.77	0.48
1:B:48:LEU:HD12	1:B:48:LEU:O	2.13	0.48
1:B:165:LYS:O	1:B:166:MET:HB2	2.11	0.48
1:D:79:ASP:C	1:D:81:ARG:N	2.66	0.48
1:E:74:TYR:CD1	1:E:74:TYR:C	2.86	0.48
1:A:54:TYR:CD1	1:A:122:SER:HB3	2.48	0.48
1:A:203:HIS:O	1:A:206:LYS:HG3	2.14	0.48
1:A:286:LYS:HD2	2:R:29:G:OP1	2.14	0.48
1:A:326:SER:OG	1:B:343:ASP:HB2	2.14	0.48
1:B:122:SER:O	1:B:123:ASP:CB	2.55	0.48
1:C:249:ILE:CD1	1:C:258:MET:HG3	2.43	0.48
1:D:164:CYS:CA	1:D:168:ASN:HB3	2.42	0.48
1:A:175:VAL:HG13	1:A:181:ILE:HG23	1.96	0.48
1:B:376:VAL:HG13	1:C:354:LYS:HB2	1.96	0.48
1:C:54:TYR:CD1	1:C:122:SER:HB3	2.48	0.48
1:D:136:LEU:HB2	1:D:213:PHE:CD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:ALA:O	1:D:401:VAL:HG22	2.13	0.48
1:E:74:TYR:O	1:E:74:TYR:HD1	1.97	0.48
1:E:323:GLU:O	1:E:327:LEU:HB2	2.14	0.48
1:A:79:ASP:C	1:A:81:ARG:N	2.67	0.48
1:B:56:TYR:CE1	1:B:126:ARG:NE	2.82	0.48
1:B:312:ARG:HG3	2:R:23:G:C5	2.49	0.48
1:D:213:PHE:O	1:D:215:TYR:N	2.46	0.48
1:E:6:LYS:HZ3	1:E:11:ASN:HD21	1.62	0.48
1:A:15:VAL:O	1:A:17:LYS:HG2	2.14	0.48
1:A:72:TYR:CE1	1:A:134:LEU:HB3	2.48	0.48
1:A:226:ALA:O	1:A:227:ALA:C	2.51	0.48
1:A:226:ALA:HB3	1:A:291:SER:HB3	1.96	0.48
1:A:269:ASP:HB3	1:E:17:LYS:HB2	1.95	0.48
1:B:129:ALA:HB1	1:B:133:TRP:HE1	1.78	0.48
1:C:317:ARG:NH1	1:C:317:ARG:N	2.60	0.48
1:C:344:LEU:O	1:C:345:ALA:CB	2.60	0.48
1:E:189:SER:O	1:E:193:LYS:HG3	2.14	0.48
1:A:74:TYR:CD1	1:A:74:TYR:C	2.87	0.48
1:A:117:LEU:N	1:A:117:LEU:CD2	2.77	0.48
1:A:359:ASP:C	1:A:361:THR:N	2.61	0.48
1:B:172:GLU:H	1:B:173:PRO:CD	2.26	0.48
1:B:189:SER:O	1:B:193:LYS:HG3	2.14	0.48
1:C:97:LYS:HB2	1:C:97:LYS:NZ	2.29	0.48
1:D:243:GLU:O	1:D:247:THR:HG23	2.14	0.48
1:A:133:TRP:CB	1:A:167:ILE:HG21	2.43	0.48
1:D:267:GLU:OE1	1:D:273:SER:HB2	2.14	0.48
1:E:233:HIS:CD2	1:E:312:ARG:HD2	2.48	0.48
1:A:25:VAL:HG11	1:A:288:PRO:HA	1.96	0.48
1:A:247:THR:HA	1:B:348:PHE:HB2	1.95	0.48
1:E:162:ASN:HA	1:E:165:LYS:NZ	2.28	0.48
1:A:383:GLU:HG3	1:B:354:LYS:HE2	1.96	0.47
1:B:182:PHE:HB2	1:B:185:TRP:CE2	2.48	0.47
1:B:215:TYR:C	1:B:215:TYR:CD2	2.88	0.47
1:C:175:VAL:HG13	1:C:181:ILE:HG23	1.96	0.47
1:D:31:TYR:C	1:D:31:TYR:CD1	2.87	0.47
1:D:143:ARG:HH22	2:R:8:G:C3’	2.18	0.47
1:E:192:THR:HA	1:E:195:VAL:CG1	2.44	0.47
1:E:218:ILE:C	1:E:220:SER:H	2.18	0.47
1:D:74:TYR:HD1	1:D:74:TYR:C	2.17	0.47
1:E:74:TYR:C	1:E:74:TYR:HD1	2.17	0.47
1:E:117:LEU:N	1:E:117:LEU:CD2	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:PHE:O	1:B:225:CYS:HB2	2.14	0.47
1:D:177:GLU:HG2	1:D:181:ILE:HD11	1.96	0.47
1:D:261:MET:HE3	1:D:297:PHE:CG	2.50	0.47
1:D:261:MET:HE3	1:D:297:PHE:CD2	2.50	0.47
1:B:126:ARG:HH11	1:B:127:THR:HG22	1.78	0.47
1:D:97:LYS:HB2	1:D:97:LYS:NZ	2.30	0.47
1:D:152:TYR:CE1	1:D:153:ARG:NH1	2.82	0.47
1:E:215:TYR:C	1:E:215:TYR:CD2	2.87	0.47
1:A:79:ASP:HB2	1:A:81:ARG:NE	2.29	0.47
1:B:153:ARG:HH21	1:B:156:LEU:CD1	2.28	0.47
1:B:253:GLU:CD	1:B:253:GLU:H	2.17	0.47
1:D:45:THR:CB	1:D:111:LYS:HZ2	2.27	0.47
1:A:317:ARG:CZ	2:R:32:G:OP2	2.63	0.47
1:B:57:GLN:C	1:B:59:LEU:N	2.68	0.47
1:C:143:ARG:HH22	2:R:17:G:H2'	1.77	0.47
1:D:129:ALA:HB1	1:D:133:TRP:HE1	1.79	0.47
1:D:286:LYS:HE3	2:R:3:G:OP2	2.14	0.47
1:E:79:ASP:HB2	1:E:81:ARG:NE	2.30	0.47
1:E:79:ASP:C	1:E:81:ARG:N	2.68	0.47
1:E:227:ALA:O	1:E:229:ALA:N	2.48	0.47
1:B:25:VAL:HG11	1:B:288:PRO:HA	1.97	0.47
1:C:38:ILE:HD12	1:C:38:ILE:O	2.14	0.47
1:E:160:LEU:HD12	1:E:160:LEU:O	2.15	0.47
1:A:169:GLU:HA	1:A:170:GLN:CD	2.35	0.47
1:A:267:GLU:OE1	1:A:273:SER:HB2	2.15	0.47
1:A:359:ASP:HB3	1:A:361:THR:OG1	2.15	0.47
1:B:143:ARG:HH22	2:R:26:G:H2'	1.79	0.47
1:C:81:ARG:HD2	1:C:208:HIS:CE1	2.49	0.47
1:C:344:LEU:N	1:C:344:LEU:CD2	2.77	0.47
1:E:295:PRO:HB2	1:E:322:ILE:CG2	2.45	0.47
2:R:9:G:H2'	2:R:10:G:O4'	2.15	0.47
1:A:29:ALA:C	1:A:31:TYR:N	2.68	0.47
1:B:107:LEU:HD23	1:B:274:TYR:HE2	1.79	0.47
1:C:126:ARG:HH11	1:C:127:THR:HG22	1.80	0.47
2:R:28:G:C8	2:R:29:G:N7	2.83	0.47
1:A:89:SER:O	1:A:90:SER:HB2	2.15	0.46
1:A:249:ILE:HD11	1:A:258:MET:HG3	1.98	0.46
1:B:141:LEU:HD12	1:B:185:TRP:CH2	2.49	0.46
1:B:412:ILE:C	1:B:412:ILE:HD12	2.35	0.46
1:C:79:ASP:C	1:C:81:ARG:N	2.68	0.46
1:C:152:TYR:HE1	1:C:153:ARG:NH1	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:GLN:HG2	1:C:171:PHE:H	1.80	0.46
1:D:31:TYR:CD1	1:D:32:PHE:N	2.83	0.46
1:D:107:LEU:HD23	1:D:274:TYR:HE2	1.80	0.46
1:E:249:ILE:CD1	1:E:258:MET:HG3	2.45	0.46
1:E:302:GLN:HG2	1:E:316:ALA:CB	2.45	0.46
1:A:215:TYR:HD1	2:R:36:G:C8	2.33	0.46
1:B:18:LEU:HD12	1:C:232:GLY:HA3	1.94	0.46
1:B:261:MET:HE3	1:B:297:PHE:CD2	2.50	0.46
1:C:130:ASP:C	1:C:132:LYS:N	2.66	0.46
1:E:25:VAL:HG11	1:E:288:PRO:HA	1.97	0.46
1:E:126:ARG:HD3	1:E:127:THR:H	1.79	0.46
1:E:136:LEU:HB2	1:E:213:PHE:CE2	2.50	0.46
1:A:179:ARG:HA	1:A:183:ASP:HB2	1.97	0.46
1:B:175:VAL:CG2	1:B:176:PRO:O	2.63	0.46
1:E:226:ALA:HB3	1:E:291:SER:HB3	1.95	0.46
1:E:233:HIS:HB2	1:E:312:ARG:NH1	2.30	0.46
1:A:28:PRO:HD2	1:A:266:GLN:NE2	2.31	0.46
1:B:152:TYR:CE1	1:B:177:GLU:HG3	2.49	0.46
1:B:160:LEU:HD12	1:B:160:LEU:O	2.15	0.46
1:C:189:SER:O	1:C:193:LYS:HG3	2.16	0.46
1:C:218:ILE:HG23	1:C:219:VAL:N	2.30	0.46
1:C:249:ILE:HD11	1:C:258:MET:HG3	1.98	0.46
1:C:412:ILE:HD12	1:C:412:ILE:C	2.36	0.46
1:D:200:MET:HB2	1:D:277:TYR:CE2	2.50	0.46
1:E:111:LYS:HE2	1:E:111:LYS:HB3	1.68	0.46
1:E:317:ARG:CG	2:R:40:G:C5	2.99	0.46
2:R:5:G:C2	2:R:7:G:H1’	2.51	0.46
1:B:179:ARG:HA	1:B:183:ASP:HB2	1.97	0.46
1:B:187:ASN:OD1	1:C:165:LYS:HE3	2.14	0.46
1:B:203:HIS:O	1:B:206:LYS:HG3	2.16	0.46
1:C:25:VAL:HG11	1:C:288:PRO:HA	1.98	0.46
1:D:218:ILE:HG23	1:D:219:VAL:N	2.30	0.46
1:E:81:ARG:HB3	1:E:208:HIS:HE2	1.80	0.46
1:B:43:ASN:HA	1:B:112:ALA:N	2.12	0.46
1:B:89:SER:O	1:B:90:SER:HB2	2.15	0.46
1:B:249:ILE:CD1	1:B:258:MET:HG3	2.45	0.46
1:B:286:LYS:HE2	1:B:293:LYS:HD3	1.96	0.46
1:C:228:LEU:O	1:C:228:LEU:HD13	2.16	0.46
1:D:57:GLN:C	1:D:59:LEU:N	2.69	0.46
1:E:29:ALA:C	1:E:31:TYR:N	2.69	0.46
1:E:104:ILE:HD13	1:E:198:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HB3	1:A:170:GLN:NE2	2.31	0.46
2:R:11:G:H2'	2:R:12:G:O4'	2.15	0.46
1:A:103:GLY:N	1:A:106:ASP:OD2	2.40	0.46
1:B:74:TYR:CD1	1:B:74:TYR:C	2.88	0.46
1:B:136:LEU:HB2	1:B:213:PHE:CD2	2.50	0.46
1:B:352:ASP:OD1	1:B:352:ASP:O	2.34	0.46
1:C:15:VAL:O	1:C:17:LYS:HG2	2.16	0.46
1:C:215:TYR:C	1:C:215:TYR:CD2	2.89	0.46
1:A:46:LYS:HA	1:A:46:LYS:HD3	1.57	0.46
1:A:72:TYR:HE1	1:A:134:LEU:HD12	1.75	0.46
1:A:74:TYR:C	1:A:74:TYR:HD1	2.19	0.46
1:A:133:TRP:HB3	1:A:167:ILE:CG1	2.45	0.46
1:A:133:TRP:HB3	1:A:167:ILE:HG12	1.98	0.46
1:A:134:LEU:HA	1:A:134:LEU:HD22	1.80	0.46
1:A:152:TYR:CD1	1:A:177:GLU:HG3	2.51	0.46
1:A:228:LEU:O	1:A:228:LEU:HD13	2.15	0.46
1:B:38:ILE:HD11	1:B:107:LEU:O	2.15	0.46
1:B:141:LEU:HB3	1:B:182:PHE:CD1	2.51	0.46
1:B:257:GLU:O	1:B:261:MET:HG3	2.16	0.46
1:B:302:GLN:HG2	1:B:316:ALA:CB	2.46	0.46
1:C:356:THR:CG2	1:C:357:PRO:HD3	2.41	0.46
1:D:153:ARG:HE	1:D:156:LEU:HD13	1.80	0.46
1:D:213:PHE:C	1:D:215:TYR:H	2.19	0.46
2:R:34:G:H4'	2:R:34:G:OP2	2.15	0.46
1:A:130:ASP:C	1:A:132:LYS:N	2.69	0.46
1:A:358:ASP:CG	1:A:359:ASP:N	2.69	0.46
1:B:408:ARG:HD3	2:R:24:G:N7	2.31	0.46
1:C:46:LYS:HD3	1:C:46:LYS:HA	1.49	0.46
1:C:160:LEU:O	1:C:160:LEU:HD12	2.16	0.46
1:C:317:ARG:NH2	2:R:13:G:O2'	2.48	0.46
1:D:46:LYS:HA	1:D:46:LYS:HD3	1.62	0.46
1:D:56:TYR:CE1	1:D:126:ARG:NH2	2.84	0.46
1:A:6:LYS:NZ	1:A:11:ASN:HD21	2.14	0.45
1:A:133:TRP:CB	1:A:167:ILE:HD13	2.46	0.45
1:A:143:ARG:HE	1:A:155:LYS:HZ1	1.64	0.45
1:B:323:GLU:O	1:B:327:LEU:HB2	2.15	0.45
1:D:194:ILE:O	1:D:198:VAL:HG23	2.16	0.45
1:D:249:ILE:CD1	1:D:258:MET:HG3	2.47	0.45
1:E:243:GLU:O	1:E:247:THR:HG23	2.16	0.45
1:A:20:ALA:O	1:A:21:ASN:HB2	2.17	0.45
1:A:218:ILE:C	1:A:220:SER:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ILE:HD12	1:A:412:ILE:C	2.37	0.45
1:B:29:ALA:C	1:B:31:TYR:N	2.70	0.45
1:B:74:TYR:HD1	1:B:74:TYR:C	2.20	0.45
1:B:79:ASP:HB2	1:B:81:ARG:NE	2.31	0.45
1:D:79:ASP:O	1:D:79:ASP:OD1	2.33	0.45
1:D:136:LEU:HD23	1:D:136:LEU:C	2.37	0.45
1:E:409:GLU:O	1:E:410:LYS:HB2	2.15	0.45
1:B:343:ASP:H	1:B:344:LEU:CD2	2.29	0.45
1:C:56:TYR:CE1	1:C:126:ARG:NE	2.84	0.45
1:C:81:ARG:HB3	1:C:208:HIS:HE2	1.80	0.45
1:C:179:ARG:HA	1:C:183:ASP:HB2	1.97	0.45
1:D:56:TYR:HE1	1:D:126:ARG:NH2	2.14	0.45
1:D:179:ARG:HA	1:D:183:ASP:CG	2.37	0.45
1:D:365:THR:CG2	1:D:366:THR:H	2.26	0.45
1:A:129:ALA:O	1:A:133:TRP:NE1	2.50	0.45
1:B:218:ILE:O	1:B:220:SER:N	2.49	0.45
1:C:31:TYR:HD1	1:C:32:PHE:N	2.15	0.45
1:C:105:PHE:C	1:C:107:LEU:N	2.68	0.45
1:D:152:TYR:HE1	1:D:153:ARG:NH1	2.12	0.45
1:D:299:PHE:CZ	1:D:328:THR:HG22	2.51	0.45
1:E:38:ILE:HD11	1:E:107:LEU:O	2.17	0.45
1:E:228:LEU:O	1:E:228:LEU:HD13	2.17	0.45
1:A:299:PHE:CZ	1:A:328:THR:HG22	2.52	0.45
1:B:218:ILE:HG23	1:B:219:VAL:N	2.32	0.45
1:C:57:GLN:C	1:C:59:LEU:N	2.70	0.45
1:C:152:TYR:CE1	1:C:153:ARG:NH1	2.84	0.45
1:C:273:SER:OG	1:C:274:TYR:N	2.47	0.45
1:D:182:PHE:HB2	1:D:185:TRP:CE2	2.52	0.45
1:E:79:ASP:O	1:E:79:ASP:OD1	2.35	0.45
1:E:172:GLU:CB	1:E:173:PRO:CD	2.83	0.45
2:R:6:G:C8	2:R:6:G:C3'	2.99	0.45
1:A:218:ILE:HG23	1:A:219:VAL:N	2.32	0.45
1:A:222:PHE:O	1:A:225:CYS:HB2	2.17	0.45
1:B:72:TYR:HE1	1:B:134:LEU:HD12	1.76	0.45
1:C:38:ILE:CD1	1:C:107:LEU:O	2.65	0.45
1:C:295:PRO:HB2	1:C:322:ILE:CG2	2.46	0.45
1:D:127:THR:OG1	1:D:128:SER:N	2.50	0.45
1:E:31:TYR:HD1	1:E:32:PHE:N	2.15	0.45
1:E:46:LYS:HA	1:E:46:LYS:HD3	1.57	0.45
1:E:152:TYR:CD1	1:E:177:GLU:HG3	2.52	0.45
1:E:172:GLU:N	1:E:173:PRO:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:GLU:HB3	1:E:178:GLY:H	1.54	0.45
1:A:80:ILE:HA	1:A:103:GLY:CA	2.47	0.45
1:A:253:GLU:CD	1:A:253:GLU:H	2.19	0.45
1:C:79:ASP:HB2	1:C:81:ARG:NE	2.32	0.45
1:D:15:VAL:O	1:D:17:LYS:HG2	2.16	0.45
1:D:48:LEU:HD12	1:D:48:LEU:O	2.16	0.45
1:D:226:ALA:HB3	1:D:291:SER:HB3	1.98	0.45
1:A:302:GLN:HG2	1:A:316:ALA:CB	2.47	0.45
1:D:25:VAL:HG11	1:D:288:PRO:HA	1.99	0.45
1:D:28:PRO:HD2	1:D:266:GLN:NE2	2.32	0.45
1:D:107:LEU:HD23	1:D:274:TYR:OH	2.17	0.45
1:E:179:ARG:HA	1:E:183:ASP:CG	2.37	0.45
1:A:160:LEU:HD12	1:A:160:LEU:O	2.17	0.45
1:A:163:GLN:OE1	1:A:163:GLN:N	2.49	0.45
1:A:246:THR:HG22	1:B:348:PHE:CD1	2.52	0.45
1:B:176:PRO:O	1:B:181:ILE:HG13	2.11	0.45
1:C:55:VAL:HG23	1:C:56:TYR:N	2.30	0.45
1:C:162:ASN:HA	1:C:165:LYS:HZ3	1.82	0.45
1:D:152:TYR:OH	1:D:153:ARG:NH1	2.50	0.45
1:A:2:SER:O	1:B:243:GLU:HG3	2.17	0.45
1:A:359:ASP:O	1:A:361:THR:N	2.45	0.45
1:B:152:TYR:CE1	1:B:153:ARG:NH1	2.85	0.45
1:B:218:ILE:C	1:B:220:SER:N	2.68	0.45
1:C:298:HIS:CD2	1:C:317:ARG:NH1	2.85	0.45
1:D:153:ARG:HH21	1:D:156:LEU:CD1	2.29	0.45
1:D:323:GLU:O	1:D:327:LEU:HB2	2.16	0.45
1:E:6:LYS:HD2	1:E:11:ASN:OD1	2.17	0.45
1:E:126:ARG:HH11	1:E:127:THR:HG22	1.82	0.45
1:E:213:PHE:O	1:E:215:TYR:N	2.50	0.45
1:A:57:GLN:C	1:A:59:LEU:N	2.70	0.44
1:A:105:PHE:O	1:A:107:LEU:N	2.50	0.44
1:A:246:THR:HG22	1:B:348:PHE:CG	2.52	0.44
1:B:55:VAL:HG23	1:B:56:TYR:N	2.30	0.44
1:B:133:TRP:HB3	1:B:167:ILE:CD1	2.47	0.44
1:C:196:ALA:HB3	1:C:281:PHE:CE1	2.52	0.44
1:C:299:PHE:CZ	1:C:328:THR:HG22	2.52	0.44
1:D:179:ARG:HA	1:D:183:ASP:HB2	1.98	0.44
1:E:390:THR:HB	1:E:391:PRO:CD	2.47	0.44
1:A:170:GLN:HB2	1:A:171:PHE:H	1.66	0.44
1:B:79:ASP:C	1:B:81:ARG:N	2.69	0.44
1:B:149:MET:HB3	2:R:24:G:N3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:VAL:HG22	1:B:176:PRO:O	2.16	0.44
1:C:233:HIS:CD2	1:C:312:ARG:HD2	2.52	0.44
1:D:163:GLN:N	1:D:163:GLN:OE1	2.48	0.44
1:E:226:ALA:O	1:E:227:ALA:C	2.55	0.44
1:E:273:SER:OG	1:E:274:TYR:N	2.50	0.44
1:E:385:GLN:CG	1:E:390:THR:HG22	2.47	0.44
2:R:18:G:H2’	2:R:19:G:C8	2.53	0.44
1:B:40:LEU:HD11	1:B:194:ILE:HG12	2.00	0.44
1:B:267:GLU:OE1	1:B:273:SER:HB2	2.17	0.44
1:C:122:SER:O	1:C:123:ASP:CB	2.59	0.44
1:C:163:GLN:O	1:C:167:ILE:HG12	2.18	0.44
1:D:141:LEU:HB3	1:D:182:PHE:CD1	2.52	0.44
1:D:231:PHE:HB2	1:D:297:PHE:CZ	2.53	0.44
1:D:299:PHE:HZ	1:D:415:TYR:CE1	2.36	0.44
1:E:84:LEU:HB3	1:E:86:LYS:O	2.16	0.44
1:B:236:LYS:HD3	1:B:236:LYS:HA	1.84	0.44
1:D:342:ALA:CB	1:D:344:LEU:HD23	2.48	0.44
1:E:53:GLY:O	1:E:54:TYR:C	2.56	0.44
1:A:127:THR:OG1	1:A:128:SER:N	2.50	0.44
1:A:236:LYS:HD3	1:A:236:LYS:HA	1.84	0.44
1:C:104:ILE:HD13	1:C:198:VAL:HG22	2.00	0.44
1:E:45:THR:CB	1:E:111:LYS:HZ2	2.31	0.44
1:A:79:ASP:O	1:A:79:ASP:OD1	2.36	0.44
1:A:126:ARG:HH11	1:A:127:THR:HG22	1.82	0.44
1:A:215:TYR:HD1	2:R:36:G:H8	1.66	0.44
1:B:56:TYR:HE1	1:B:126:ARG:NH2	2.16	0.44
1:B:299:PHE:CZ	1:B:328:THR:HG22	2.53	0.44
1:C:241:SER:OG	1:C:243:GLU:HG2	2.16	0.44
1:D:55:VAL:HG23	1:D:56:TYR:N	2.32	0.44
1:D:175:VAL:HG13	1:D:181:ILE:HG23	1.99	0.44
1:A:81:ARG:HB3	1:A:208:HIS:HE2	1.82	0.44
1:A:164:CYS:HA	1:A:168:ASN:HA	1.98	0.44
1:A:243:GLU:HG3	1:E:2:SER:O	2.18	0.44
1:A:356:THR:CG2	1:A:357:PRO:HD3	2.42	0.44
1:B:55:VAL:O	1:B:56:TYR:C	2.56	0.44
1:B:56:TYR:CE1	1:B:126:ARG:NH2	2.86	0.44
1:B:81:ARG:HB3	1:B:208:HIS:HE2	1.82	0.44
1:B:163:GLN:OE1	1:B:163:GLN:N	2.50	0.44
1:C:56:TYR:CE1	1:C:126:ARG:NH2	2.85	0.44
1:C:302:GLN:HG2	1:C:316:ALA:CB	2.47	0.44
1:D:164:CYS:HB3	1:D:168:ASN:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ILE:C	1:D:220:SER:H	2.21	0.44
1:D:302:GLN:HG2	1:D:316:ALA:CB	2.48	0.44
1:E:57:GLN:NE2	1:E:60:LYS:HZ2	1.82	0.44
1:E:247:THR:O	1:E:375:VAL:HG11	2.18	0.44
1:A:243:GLU:HG2	1:A:243:GLU:H	1.47	0.44
1:B:226:ALA:O	1:B:227:ALA:C	2.56	0.44
1:C:20:ALA:O	1:C:21:ASN:HB2	2.18	0.44
1:C:233:HIS:HB2	1:C:312:ARG:HH11	1.82	0.44
1:C:236:LYS:HD3	1:C:236:LYS:HA	1.83	0.44
1:D:352:ASP:OD1	1:D:352:ASP:O	2.36	0.44
1:D:390:THR:HB	1:D:391:PRO:CD	2.48	0.44
1:E:241:SER:OG	1:E:243:GLU:HG2	2.16	0.44
1:E:243:GLU:H	1:E:243:GLU:HG2	1.50	0.44
1:B:152:TYR:HE1	1:B:153:ARG:NH1	2.15	0.44
1:C:134:LEU:N	1:C:135:PRO:CD	2.80	0.44
1:E:105:PHE:C	1:E:107:LEU:N	2.69	0.44
1:A:153:ARG:HH21	1:A:156:LEU:CD1	2.31	0.43
1:B:130:ASP:C	1:B:132:LYS:N	2.69	0.43
1:B:171:PHE:CG	1:B:172:GLU:N	2.85	0.43
1:C:29:ALA:C	1:C:31:TYR:N	2.71	0.43
1:C:90:SER:HG	1:C:91:PHE:HD1	1.63	0.43
1:C:103:GLY:N	1:C:106:ASP:OD2	2.39	0.43
1:C:218:ILE:C	1:C:220:SER:H	2.21	0.43
1:E:153:ARG:HE	1:E:156:LEU:HD13	1.83	0.43
1:C:224:ASP:HB2	1:C:279:ILE:HG13	2.00	0.43
1:E:55:VAL:HG23	1:E:56:TYR:N	2.34	0.43
1:E:122:SER:O	1:E:123:ASP:CB	2.57	0.43
1:E:141:LEU:HD12	1:E:185:TRP:CH2	2.53	0.43
1:E:179:ARG:HA	1:E:183:ASP:HB2	2.00	0.43
1:B:15:VAL:O	1:B:17:LYS:HG2	2.18	0.43
1:B:317:ARG:NE	2:R:22:G:O2'	2.51	0.43
1:C:29:ALA:H	1:C:266:GLN:HE22	1.65	0.43
1:C:177:GLU:HG2	1:C:181:ILE:CD1	2.48	0.43
1:D:54:TYR:CD1	1:D:122:SER:CB	3.01	0.43
1:E:222:PHE:O	1:E:225:CYS:HB2	2.18	0.43
1:A:55:VAL:HG23	1:A:56:TYR:N	2.31	0.43
1:A:136:LEU:HD23	1:A:136:LEU:C	2.39	0.43
1:A:152:TYR:HE1	1:A:153:ARG:NH1	2.16	0.43
1:A:227:ALA:HA	1:A:230:THR:HG23	2.00	0.43
1:B:107:LEU:C	1:B:108:VAL:HG23	2.38	0.43
1:B:249:ILE:HD11	1:B:258:MET:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:CYS:HA	1:C:168:ASN:CA	2.48	0.43
1:D:316:ALA:HA	1:D:317:ARG:HH22	1.82	0.43
1:E:152:TYR:HE1	1:E:153:ARG:NH1	2.16	0.43
1:E:175:VAL:HG13	1:E:181:ILE:HG23	2.00	0.43
1:A:172:GLU:H	1:A:173:PRO:CD	2.30	0.43
1:B:187:ASN:ND2	1:C:165:LYS:CD	2.82	0.43
1:C:179:ARG:HA	1:C:183:ASP:CG	2.38	0.43
1:C:267:GLU:OE1	1:C:273:SER:HB2	2.18	0.43
1:D:364:LEU:HD22	1:D:368:ALA:CB	2.48	0.43
1:A:66:ILE:HD13	1:A:185:TRP:CG	2.53	0.43
1:A:136:LEU:HB2	1:A:213:PHE:CD2	2.54	0.43
1:B:316:ALA:O	1:B:411:THR:HA	2.18	0.43
1:C:369:PRO:HA	1:C:370:PRO:HD3	1.86	0.43
1:E:80:ILE:HA	1:E:103:GLY:CA	2.48	0.43
1:A:149:MET:HG3	2:R:33:G:O4'	2.18	0.43
1:B:19:PRO:HD3	1:C:228:LEU:CD2	2.49	0.43
1:C:226:ALA:O	1:C:227:ALA:C	2.57	0.43
1:E:56:TYR:CE1	1:E:126:ARG:NE	2.87	0.43
1:E:127:THR:OG1	1:E:128:SER:N	2.51	0.43
2:R:27:G:N3	2:R:27:G:H5'	2.34	0.43
1:A:31:TYR:HD1	1:A:32:PHE:N	2.16	0.43
1:B:213:PHE:O	1:B:215:TYR:N	2.52	0.43
1:C:111:LYS:HB3	1:C:111:LYS:HE2	1.71	0.43
1:D:294:ASN:N	1:D:295:PRO:HD3	2.34	0.43
1:E:130:ASP:C	1:E:132:LYS:N	2.72	0.43
1:E:253:GLU:CD	1:E:253:GLU:H	2.20	0.43
1:E:298:HIS:CD2	1:E:317:ARG:NH1	2.86	0.43
1:E:299:PHE:CZ	1:E:328:THR:HG22	2.54	0.43
1:E:358:ASP:CG	1:E:359:ASP:N	2.71	0.43
2:R:6:G:O5'	2:R:6:G:H8	2.02	0.43
1:A:111:LYS:HB3	1:A:111:LYS:HE2	1.73	0.43
1:A:218:ILE:O	1:A:220:SER:N	2.51	0.43
1:C:56:TYR:HE1	1:C:126:ARG:NH2	2.17	0.43
1:D:107:LEU:C	1:D:108:VAL:HG23	2.39	0.43
1:D:111:LYS:HE2	1:D:111:LYS:HB3	1.67	0.43
1:D:241:SER:OG	1:D:243:GLU:HG2	2.17	0.43
1:A:56:TYR:CE1	1:A:126:ARG:NE	2.86	0.43
1:A:133:TRP:CD1	1:A:167:ILE:HG23	2.54	0.43
1:C:323:GLU:O	1:C:327:LEU:HB2	2.18	0.43
1:C:342:ALA:HB3	1:C:344:LEU:HD23	2.01	0.43
1:D:81:ARG:HB3	1:D:208:HIS:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:17:G:HO2'	2:R:18:G:P	2.42	0.43
1:A:323:GLU:O	1:A:327:LEU:HB2	2.19	0.42
1:B:175:VAL:HG13	1:B:181:ILE:HG23	2.01	0.42
1:D:52:ARG:O	1:D:55:VAL:HG23	2.19	0.42
1:A:6:LYS:HZ3	1:A:11:ASN:HD21	1.67	0.42
1:A:385:GLN:CG	1:A:390:THR:HG22	2.46	0.42
1:B:31:TYR:HD1	1:B:32:PHE:N	2.16	0.42
1:B:213:PHE:C	1:B:215:TYR:H	2.23	0.42
1:B:241:SER:OG	1:B:243:GLU:HG2	2.19	0.42
1:B:307:LEU:HD12	1:B:307:LEU:HA	1.85	0.42
1:C:136:LEU:HB2	1:C:213:PHE:CD2	2.54	0.42
1:E:28:PRO:HD2	1:E:266:GLN:NE2	2.34	0.42
1:E:213:PHE:C	1:E:215:TYR:H	2.23	0.42
2:R:18:G:H3'	2:R:19:G:C8	2.54	0.42
2:R:27:G:H3'	2:R:28:G:C8	2.53	0.42
1:A:171:PHE:O	1:A:172:GLU:OE2	2.36	0.42
1:A:352:ASP:OD1	1:A:352:ASP:O	2.37	0.42
1:B:57:GLN:C	1:B:59:LEU:H	2.23	0.42
1:B:117:LEU:N	1:B:117:LEU:CD2	2.81	0.42
1:C:285:SER:HB3	1:D:207:LYS:NZ	2.35	0.42
1:D:6:LYS:NZ	1:D:11:ASN:HD21	2.17	0.42
1:D:177:GLU:HG2	1:D:181:ILE:CD1	2.49	0.42
1:D:195:VAL:HG23	1:D:217:THR:OG1	2.19	0.42
1:D:254:VAL:HG13	1:D:297:PHE:HA	2.01	0.42
1:A:134:LEU:N	1:A:135:PRO:CD	2.81	0.42
1:A:270:LYS:HE2	1:A:270:LYS:HB3	1.83	0.42
1:B:57:GLN:O	1:B:59:LEU:N	2.52	0.42
1:B:105:PHE:C	1:B:107:LEU:N	2.70	0.42
1:B:343:ASP:C	1:B:344:LEU:HD22	2.40	0.42
1:C:107:LEU:HD23	1:C:274:TYR:OH	2.19	0.42
1:C:149:MET:HG3	2:R:15:G:C8	2.55	0.42
1:C:285:SER:OG	1:D:207:LYS:HE2	2.19	0.42
1:D:38:ILE:HA	1:D:39:PRO:HD2	1.87	0.42
1:D:344:LEU:O	1:D:345:ALA:CB	2.68	0.42
1:A:227:ALA:C	1:A:229:ALA:N	2.73	0.42
1:A:261:MET:HE3	1:A:297:PHE:CG	2.55	0.42
1:B:247:THR:HA	1:C:348:PHE:HB2	2.01	0.42
1:D:38:ILE:HD11	1:D:107:LEU:O	2.19	0.42
1:E:38:ILE:HD12	1:E:38:ILE:O	2.20	0.42
1:E:316:ALA:HB1	1:E:317:ARG:NH1	2.33	0.42
1:A:152:TYR:CE1	1:A:153:ARG:NH1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:HE	1:A:156:LEU:HD13	1.84	0.42
1:B:17:LYS:HG3	1:C:268:ILE:HD11	2.02	0.42
1:B:171:PHE:CD1	1:B:172:GLU:N	2.87	0.42
1:B:273:SER:OG	1:B:274:TYR:N	2.53	0.42
1:B:356:THR:CG2	1:B:357:PRO:HD3	2.44	0.42
2:R:30:G:H2'	2:R:31:G:C1'	2.49	0.42
1:A:66:ILE:HA	1:A:69:VAL:HG22	2.02	0.42
1:A:84:LEU:HB3	1:A:86:LYS:O	2.19	0.42
1:A:179:ARG:HA	1:A:183:ASP:CG	2.39	0.42
1:B:20:ALA:O	1:B:21:ASN:HB2	2.20	0.42
1:C:57:GLN:O	1:C:59:LEU:N	2.53	0.42
1:C:153:ARG:HE	1:C:156:LEU:HD13	1.83	0.42
1:C:375:VAL:O	1:C:379:LEU:HB2	2.20	0.42
1:D:257:GLU:O	1:D:261:MET:HG3	2.19	0.42
1:E:317:ARG:HE	2:R:40:G:H3'	1.84	0.42
1:A:55:VAL:O	1:A:56:TYR:C	2.58	0.42
1:A:74:TYR:O	1:A:74:TYR:HD1	2.02	0.42
1:A:112:ALA:O	1:A:113:LEU:O	2.38	0.42
1:A:355:TYR:HD2	1:A:355:TYR:HA	1.74	0.42
1:B:6:LYS:NZ	1:B:11:ASN:HD21	2.17	0.42
1:C:149:MET:O	1:C:151:GLU:N	2.53	0.42
1:D:134:LEU:HD22	1:D:134:LEU:HA	1.78	0.42
1:A:31:TYR:C	1:A:33:ARG:H	2.23	0.42
1:A:143:ARG:HD2	1:A:216:GLY:HA2	2.02	0.42
1:B:136:LEU:HD23	1:B:136:LEU:C	2.39	0.42
1:B:179:ARG:HA	1:B:183:ASP:CG	2.39	0.42
1:B:224:ASP:HB2	1:B:279:ILE:HG13	2.02	0.42
1:B:261:MET:HE3	1:B:297:PHE:CG	2.55	0.42
1:C:80:ILE:HA	1:C:103:GLY:CA	2.50	0.42
1:C:141:LEU:HD12	1:C:185:TRP:CH2	2.54	0.42
1:D:385:GLN:O	1:D:386:ASN:CB	2.68	0.42
1:E:134:LEU:HD22	1:E:134:LEU:HA	1.84	0.42
1:A:56:TYR:CE1	1:A:126:ARG:NH2	2.88	0.42
1:E:48:LEU:O	1:E:48:LEU:HD12	2.20	0.42
1:E:153:ARG:HH21	1:E:156:LEU:CD1	2.33	0.42
1:A:224:ASP:HB2	1:A:279:ILE:HG13	2.02	0.41
1:B:66:ILE:HA	1:B:69:VAL:HG22	2.02	0.41
1:C:177:GLU:HB3	1:C:178:GLY:H	1.72	0.41
1:D:270:LYS:HB3	1:D:270:LYS:HE2	1.79	0.41
1:E:56:TYR:CE1	1:E:126:ARG:NH2	2.88	0.41
1:E:57:GLN:C	1:E:59:LEU:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:LYS:O	1:E:158:ASP:OD1	2.38	0.41
1:E:257:GLU:O	1:E:261:MET:HG3	2.19	0.41
1:E:369:PRO:HA	1:E:370:PRO:HD3	1.80	0.41
1:B:80:ILE:HA	1:B:103:GLY:CA	2.50	0.41
1:B:127:THR:OG1	1:B:128:SER:N	2.53	0.41
1:C:127:THR:OG1	1:C:128:SER:N	2.54	0.41
1:E:90:SER:HG	1:E:91:PHE:HD1	1.66	0.41
1:E:141:LEU:HB3	1:E:182:PHE:CD1	2.54	0.41
1:E:218:ILE:C	1:E:220:SER:N	2.73	0.41
1:E:261:MET:HE3	1:E:297:PHE:CG	2.55	0.41
1:E:358:ASP:OD2	1:E:359:ASP:N	2.50	0.41
1:A:141:LEU:HB3	1:A:182:PHE:CD1	2.56	0.41
1:A:167:ILE:O	1:A:168:ASN:HB2	2.20	0.41
1:A:383:GLU:HG3	1:B:354:LYS:NZ	2.34	0.41
1:B:93:ILE:HD12	1:B:93:ILE:H	1.84	0.41
1:B:298:HIS:CD2	1:B:317:ARG:NH1	2.88	0.41
1:C:182:PHE:HB2	1:C:185:TRP:CE2	2.55	0.41
1:C:213:PHE:O	1:C:215:TYR:N	2.53	0.41
1:C:261:MET:HE3	1:C:297:PHE:CD2	2.55	0.41
1:E:136:LEU:HD23	1:E:136:LEU:C	2.41	0.41
1:A:290:SER:HA	2:R:31:G:OP1	2.20	0.41
1:B:175:VAL:HG22	1:B:181:ILE:HG23	2.02	0.41
1:C:153:ARG:HH21	1:C:156:LEU:CD1	2.34	0.41
1:C:184:VAL:HG13	1:D:165:LYS:CG	2.50	0.41
1:D:53:GLY:O	1:D:54:TYR:C	2.59	0.41
1:E:40:LEU:HD11	1:E:194:ILE:HG12	2.02	0.41
1:E:107:LEU:C	1:E:108:VAL:HG23	2.40	0.41
1:A:42:ILE:N	1:A:42:ILE:HD13	2.36	0.41
1:B:257:GLU:OE1	1:B:295:PRO:HD2	2.20	0.41
1:C:222:PHE:O	1:C:225:CYS:HB2	2.20	0.41
1:D:57:GLN:OE1	1:D:123:ASP:CB	2.68	0.41
1:E:66:ILE:HD13	1:E:185:TRP:CG	2.55	0.41
2:R:7:G:C2	2:R:8:G:C4	3.08	0.41
1:A:53:GLY:O	1:A:54:TYR:C	2.59	0.41
1:A:170:GLN:CD	1:A:170:GLN:N	2.74	0.41
1:C:200:MET:HB2	1:C:277:TYR:CE2	2.56	0.41
1:C:212:SER:HB2	2:R:18:G:C5	2.55	0.41
1:C:285:SER:CB	1:D:207:LYS:NZ	2.84	0.41
1:C:307:LEU:HD12	1:C:307:LEU:HA	1.92	0.41
1:D:154:LYS:O	1:D:158:ASP:OD1	2.38	0.41
1:D:227:ALA:C	1:D:229:ALA:N	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:ASP:C	1:E:107:LEU:HD12	2.41	0.41
1:E:149:MET:HG3	2:R:42:G:C8	2.55	0.41
1:E:155:LYS:O	1:E:159:GLY:N	2.48	0.41
1:B:84:LEU:HB3	1:B:86:LYS:O	2.20	0.41
1:B:385:GLN:CG	1:B:390:THR:HG22	2.48	0.41
1:C:6:LYS:NZ	1:C:11:ASN:HD21	2.18	0.41
1:C:255:ALA:O	1:C:259:VAL:HG23	2.21	0.41
1:D:66:ILE:HD13	1:D:185:TRP:CG	2.56	0.41
1:D:215:TYR:HA	2:R:9:G:O4’	2.20	0.41
1:D:298:HIS:CD2	1:D:317:ARG:NH1	2.88	0.41
1:D:385:GLN:CG	1:D:390:THR:HG22	2.49	0.41
1:E:182:PHE:HB2	1:E:185:TRP:CE2	2.56	0.41
1:A:38:ILE:HD12	1:A:38:ILE:O	2.21	0.41
1:C:136:LEU:HD23	1:C:136:LEU:C	2.40	0.41
1:C:257:GLU:O	1:C:261:MET:HG3	2.21	0.41
1:C:294:ASN:N	1:C:295:PRO:HD3	2.36	0.41
1:D:57:GLN:O	1:D:59:LEU:N	2.54	0.41
1:D:101:THR:O	1:D:101:THR:HG22	2.21	0.41
1:D:175:VAL:HG22	1:D:176:PRO:O	2.19	0.41
1:D:228:LEU:O	1:D:228:LEU:HD13	2.20	0.41
1:E:143:ARG:HH22	2:R:44:G:H5”	1.85	0.41
1:E:215:TYR:CD1	2:R:45:G:H5”	2.56	0.41
1:A:60:LYS:HB2	1:A:60:LYS:HE2	1.85	0.41
1:A:316:ALA:HB1	1:A:317:ARG:NH1	2.31	0.41
1:A:344:LEU:N	1:A:344:LEU:HD22	2.35	0.41
1:A:344:LEU:HD11	1:E:330:ALA:CB	2.50	0.41
1:B:38:ILE:HA	1:B:39:PRO:HD2	1.86	0.41
1:B:53:GLY:O	1:B:54:TYR:C	2.59	0.41
1:C:28:PRO:HD2	1:C:266:GLN:NE2	2.35	0.41
1:C:130:ASP:C	1:C:132:LYS:H	2.24	0.41
1:C:200:MET:SD	1:C:274:TYR:CD2	3.14	0.41
1:C:409:GLU:O	1:C:410:LYS:HB2	2.21	0.41
1:D:117:LEU:N	1:D:117:LEU:CD2	2.82	0.41
1:D:141:LEU:HD12	1:D:185:TRP:CH2	2.55	0.41
1:E:38:ILE:HA	1:E:39:PRO:HD2	1.83	0.41
1:E:152:TYR:CE1	1:E:153:ARG:NH1	2.88	0.41
1:A:56:TYR:HE1	1:A:126:ARG:NH2	2.19	0.41
1:A:90:SER:HG	1:A:91:PHE:HD1	1.68	0.41
1:A:171:PHE:CG	1:A:172:GLU:N	2.88	0.41
1:A:200:MET:SD	1:A:274:TYR:HD2	2.44	0.41
1:A:257:GLU:HG2	1:A:294:ASN:HA	2.03	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:354:LYS:HZ3	1:E:380:GLY:HA2	1.85	0.41
1:C:93:ILE:H	1:C:93:ILE:HD12	1.85	0.41
1:C:165:LYS:HD2	2:R:18:G:O6	2.20	0.41
1:D:54:TYR:HD1	1:D:122:SER:HB3	1.85	0.41
1:D:84:LEU:HB3	1:D:86:LYS:O	2.20	0.41
1:E:270:LYS:HE2	1:E:270:LYS:HB3	1.85	0.41
1:E:402:MET:O	1:E:403:SER:OG	2.31	0.41
1:A:261:MET:HE3	1:A:297:PHE:CD2	2.55	0.40
1:B:233:HIS:CD2	1:B:312:ARG:HD2	2.55	0.40
1:C:312:ARG:HG3	2:R:14:G:C6	2.56	0.40
1:D:130:ASP:C	1:D:132:LYS:N	2.73	0.40
1:D:342:ALA:HB3	1:D:344:LEU:HD23	2.01	0.40
1:D:365:THR:CG2	1:D:366:THR:N	2.82	0.40
1:D:369:PRO:HA	1:D:370:PRO:HD3	1.83	0.40
1:D:375:VAL:O	1:D:379:LEU:HB2	2.21	0.40
1:E:143:ARG:NH2	2:R:44:G:H3'	2.21	0.40
1:A:40:LEU:HD11	1:A:194:ILE:HG12	2.03	0.40
1:A:182:PHE:HB2	1:A:185:TRP:CE2	2.56	0.40
1:B:143:ARG:HE	1:B:155:LYS:NZ	2.18	0.40
1:B:227:ALA:C	1:B:229:ALA:N	2.74	0.40
1:B:390:THR:HB	1:B:391:PRO:CD	2.51	0.40
1:C:6:LYS:HD2	1:C:11:ASN:OD1	2.22	0.40
1:C:133:TRP:CH2	1:C:134:LEU:HD23	2.57	0.40
1:D:143:ARG:HE	1:D:155:LYS:NZ	2.15	0.40
1:D:247:THR:O	1:D:375:VAL:HG11	2.21	0.40
1:D:408:ARG:NH1	2:R:6:G:N7	2.69	0.40
1:E:54:TYR:CD1	1:E:122:SER:CB	3.04	0.40
1:E:218:ILE:HG23	1:E:219:VAL:N	2.37	0.40
1:E:224:ASP:CG	2:R:39:G:H4'	2.42	0.40
1:A:224:ASP:HA	2:R:30:G:O3'	2.22	0.40
1:A:231:PHE:HB2	1:A:297:PHE:CZ	2.56	0.40
1:A:390:THR:HB	1:A:391:PRO:CD	2.51	0.40
1:C:317:ARG:H	1:C:317:ARG:NE	2.12	0.40
1:C:419:GLU:O	1:C:419:GLU:HG3	2.22	0.40
1:D:126:ARG:HH11	1:D:127:THR:HG22	1.83	0.40
1:D:177:GLU:HB3	1:D:178:GLY:H	1.67	0.40
1:D:356:THR:CG2	1:D:357:PRO:HD3	2.45	0.40
1:E:136:LEU:HB2	1:E:213:PHE:CD2	2.56	0.40
1:A:154:LYS:O	1:A:158:ASP:OD1	2.39	0.40
1:A:171:PHE:CD1	1:A:172:GLU:N	2.90	0.40
1:A:200:MET:SD	1:A:274:TYR:CD2	3.15	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:O	1:A:247:THR:HG23	2.22	0.40
1:A:375:VAL:O	1:A:379:LEU:HB2	2.22	0.40
1:A:376:VAL:HG13	1:B:354:LYS:CA	2.51	0.40
1:B:38:ILE:CD1	1:B:107:LEU:O	2.70	0.40
1:B:227:ALA:HA	1:B:230:THR:HG23	2.02	0.40
1:D:20:ALA:O	1:D:21:ASN:HB2	2.21	0.40
1:D:129:ALA:O	1:D:133:TRP:CD1	2.74	0.40
1:D:224:ASP:HB2	1:D:279:ILE:HG13	2.04	0.40
1:D:249:ILE:HD11	1:D:258:MET:HG3	2.04	0.40
1:A:19:PRO:HA	1:B:268:ILE:O	2.21	0.40
1:A:104:ILE:HD13	1:A:198:VAL:HG22	2.04	0.40
1:A:177:GLU:HG2	1:A:181:ILE:HD11	2.02	0.40
1:A:299:PHE:HZ	1:A:415:TYR:CE1	2.40	0.40
1:B:93:ILE:HD12	1:B:93:ILE:N	2.36	0.40
1:B:316:ALA:HB1	1:B:317:ARG:NH1	2.36	0.40
1:E:227:ALA:C	1:E:229:ALA:N	2.75	0.40
1:E:254:VAL:HG13	1:E:297:PHE:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/421 (100%)	319 (76%)	66 (16%)	34 (8%)	1	4
1	B	411/421 (98%)	321 (78%)	53 (13%)	37 (9%)	1	3
1	C	409/421 (97%)	312 (76%)	67 (16%)	30 (7%)	1	5
1	D	412/421 (98%)	317 (77%)	59 (14%)	36 (9%)	1	4
1	E	419/421 (100%)	322 (77%)	66 (16%)	31 (7%)	1	5
All	All	2070/2105 (98%)	1591 (77%)	311 (15%)	168 (8%)	1	4

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	113	LEU
1	A	117	LEU
1	A	167	ILE
1	A	173	PRO
1	A	174	LEU
1	A	182	PHE
1	A	358	ASP
1	A	365	THR
1	A	366	THR
1	B	63	ASN
1	B	113	LEU
1	B	117	LEU
1	B	168	ASN
1	B	170	GLN
1	B	173	PRO
1	B	174	LEU
1	B	182	PHE
1	B	228	LEU
1	B	342	ALA
1	B	345	ALA
1	C	63	ASN
1	C	113	LEU
1	C	117	LEU
1	C	173	PRO
1	C	174	LEU
1	C	182	PHE
1	C	228	LEU
1	C	345	ALA
1	D	63	ASN
1	D	113	LEU
1	D	117	LEU
1	D	165	LYS
1	D	166	MET
1	D	169	GLU
1	D	173	PRO
1	D	174	LEU
1	D	182	PHE
1	D	228	LEU
1	D	345	ALA
1	E	63	ASN
1	E	113	LEU

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Mol	Chain	Res	Type
1	E	117	LEU
1	E	182	PHE
1	E	362	GLY
1	E	365	THR
1	A	80	ILE
1	A	115	GLY
1	A	168	ASN
1	A	180	ASP
1	A	228	LEU
1	A	271	ALA
1	A	360	SER
1	B	80	ILE
1	B	115	GLY
1	B	167	ILE
1	B	176	PRO
1	B	180	ASP
1	B	271	ALA
1	C	80	ILE
1	C	108	VAL
1	C	115	GLY
1	C	167	ILE
1	C	180	ASP
1	C	214	ARG
1	C	271	ALA
1	D	80	ILE
1	D	115	GLY
1	D	180	ASP
1	D	214	ARG
1	D	271	ALA
1	E	80	ILE
1	E	115	GLY
1	E	168	ASN
1	E	180	ASP
1	E	228	LEU
1	E	271	ALA
1	E	363	GLY
1	A	90	SER
1	A	123	ASP
1	A	172	GLU
1	A	179	ARG
1	A	226	ALA
1	B	30	ASP

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Mol	Chain	Res	Type
1	B	123	ASP
1	B	172	GLU
1	B	179	ARG
1	C	30	ASP
1	C	90	SER
1	C	123	ASP
1	C	128	SER
1	C	129	ALA
1	C	168	ASN
1	D	30	ASP
1	D	123	ASP
1	D	167	ILE
1	D	179	ARG
1	E	30	ASP
1	E	90	SER
1	E	123	ASP
1	E	129	ALA
1	E	214	ARG
1	E	226	ALA
1	A	30	ASP
1	A	128	SER
1	A	129	ALA
1	A	189	SER
1	A	309	ARG
1	A	342	ALA
1	A	357	PRO
1	B	90	SER
1	B	108	VAL
1	B	129	ALA
1	B	214	ARG
1	B	226	ALA
1	C	150	PRO
1	C	179	ARG
1	D	46	LYS
1	D	90	SER
1	D	108	VAL
1	D	129	ALA
1	D	226	ALA
1	D	309	ARG
1	D	357	PRO
1	E	108	VAL
1	E	128	SER

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Mol	Chain	Res	Type
1	E	173	PRO
1	E	179	ARG
1	A	46	LYS
1	A	100	ASP
1	A	108	VAL
1	B	46	LYS
1	B	100	ASP
1	B	128	SER
1	B	309	ARG
1	B	357	PRO
1	C	131	ASP
1	C	309	ARG
1	D	79	ASP
1	D	128	SER
1	E	309	ARG
1	E	357	PRO
1	A	42	ILE
1	A	150	PRO
1	C	46	LYS
1	D	100	ASP
1	D	106	ASP
1	D	150	PRO
1	E	46	LYS
1	E	106	ASP
1	B	42	ILE
1	D	19	PRO
1	E	19	PRO
1	E	150	PRO
1	B	19	PRO
1	B	93	ILE
1	B	150	PRO
1	B	219	VAL
1	C	93	ILE
1	C	178	GLY
1	D	93	ILE
1	B	23	ASP
1	D	23	ASP
1	E	42	ILE
1	E	93	ILE
1	C	19	PRO
1	C	42	ILE
1	D	42	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	362/362 (100%)	296 (82%)	66 (18%)	1 7
1	B	358/362 (99%)	290 (81%)	68 (19%)	1 6
1	C	356/362 (98%)	289 (81%)	67 (19%)	1 6
1	D	359/362 (99%)	289 (80%)	70 (20%)	1 6
1	E	362/362 (100%)	292 (81%)	70 (19%)	1 6
All	All	1797/1810 (99%)	1456 (81%)	341 (19%)	1 6

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	11	ASN
1	A	31	TYR
1	A	40	LEU
1	A	42	ILE
1	A	46	LYS
1	A	49	SER
1	A	55	VAL
1	A	56	TYR
1	A	57	GLN
1	A	60	LYS
1	A	67	ILE
1	A	74	TYR
1	A	94	ASN
1	A	97	LYS
1	A	101	THR
1	A	108	VAL
1	A	117	LEU
1	A	121	VAL
1	A	126	ARG
1	A	131	ASP
1	A	132	LYS
1	A	134	LEU

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Mol	Chain	Res	Type
1	A	147	THR
1	A	149	MET
1	A	153	ARG
1	A	154	LYS
1	A	156	LEU
1	A	160	LEU
1	A	165	LYS
1	A	170	GLN
1	A	171	PHE
1	A	172	GLU
1	A	174	LEU
1	A	175	VAL
1	A	177	GLU
1	A	180	ASP
1	A	181	ILE
1	A	182	PHE
1	A	187	ASN
1	A	217	THR
1	A	228	LEU
1	A	230	THR
1	A	243	GLU
1	A	251	ASN
1	A	252	ARG
1	A	253	GLU
1	A	258	MET
1	A	263	LEU
1	A	268	ILE
1	A	270	LYS
1	A	272	ASP
1	A	273	SER
1	A	307	LEU
1	A	308	LEU
1	A	317	ARG
1	A	327	LEU
1	A	332	LEU
1	A	344	LEU
1	A	352	ASP
1	A	354	LYS
1	A	356	THR
1	A	361	THR
1	A	385	GLN
1	A	405	GLN

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Mol	Chain	Res	Type
1	A	409	GLU
1	B	3	VAL
1	B	11	ASN
1	B	31	TYR
1	B	40	LEU
1	B	42	ILE
1	B	46	LYS
1	B	49	SER
1	B	55	VAL
1	B	56	TYR
1	B	57	GLN
1	B	60	LYS
1	B	67	ILE
1	B	74	TYR
1	B	78	LYS
1	B	94	ASN
1	B	97	LYS
1	B	101	THR
1	B	108	VAL
1	B	117	LEU
1	B	121	VAL
1	B	128	SER
1	B	131	ASP
1	B	132	LYS
1	B	134	LEU
1	B	147	THR
1	B	149	MET
1	B	153	ARG
1	B	154	LYS
1	B	156	LEU
1	B	160	LEU
1	B	162	ASN
1	B	165	LYS
1	B	167	ILE
1	B	169	GLU
1	B	170	GLN
1	B	171	PHE
1	B	172	GLU
1	B	174	LEU
1	B	175	VAL
1	B	177	GLU
1	B	180	ASP

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Mol	Chain	Res	Type
1	B	181	ILE
1	B	182	PHE
1	B	187	ASN
1	B	217	THR
1	B	228	LEU
1	B	243	GLU
1	B	251	ASN
1	B	252	ARG
1	B	253	GLU
1	B	258	MET
1	B	263	LEU
1	B	268	ILE
1	B	270	LYS
1	B	272	ASP
1	B	273	SER
1	B	307	LEU
1	B	308	LEU
1	B	317	ARG
1	B	327	LEU
1	B	332	LEU
1	B	343	ASP
1	B	352	ASP
1	B	354	LYS
1	B	356	THR
1	B	385	GLN
1	B	405	GLN
1	B	409	GLU
1	C	3	VAL
1	C	8	ILE
1	C	11	ASN
1	C	31	TYR
1	C	40	LEU
1	C	46	LYS
1	C	49	SER
1	C	56	TYR
1	C	57	GLN
1	C	60	LYS
1	C	67	ILE
1	C	74	TYR
1	C	94	ASN
1	C	97	LYS
1	C	100	ASP

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Mol	Chain	Res	Type
1	C	101	THR
1	C	108	VAL
1	C	117	LEU
1	C	121	VAL
1	C	128	SER
1	C	131	ASP
1	C	132	LYS
1	C	134	LEU
1	C	147	THR
1	C	149	MET
1	C	153	ARG
1	C	154	LYS
1	C	156	LEU
1	C	160	LEU
1	C	165	LYS
1	C	166	MET
1	C	167	ILE
1	C	171	PHE
1	C	172	GLU
1	C	174	LEU
1	C	175	VAL
1	C	177	GLU
1	C	180	ASP
1	C	181	ILE
1	C	182	PHE
1	C	187	ASN
1	C	217	THR
1	C	228	LEU
1	C	230	THR
1	C	243	GLU
1	C	251	ASN
1	C	252	ARG
1	C	253	GLU
1	C	258	MET
1	C	263	LEU
1	C	268	ILE
1	C	270	LYS
1	C	272	ASP
1	C	273	SER
1	C	278	LEU
1	C	307	LEU
1	C	308	LEU

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Mol	Chain	Res	Type
1	C	317	ARG
1	C	327	LEU
1	C	332	LEU
1	C	343	ASP
1	C	344	LEU
1	C	352	ASP
1	C	354	LYS
1	C	356	THR
1	C	405	GLN
1	C	409	GLU
1	D	3	VAL
1	D	11	ASN
1	D	31	TYR
1	D	40	LEU
1	D	42	ILE
1	D	46	LYS
1	D	49	SER
1	D	55	VAL
1	D	56	TYR
1	D	57	GLN
1	D	60	LYS
1	D	67	ILE
1	D	74	TYR
1	D	94	ASN
1	D	97	LYS
1	D	100	ASP
1	D	101	THR
1	D	108	VAL
1	D	117	LEU
1	D	121	VAL
1	D	126	ARG
1	D	131	ASP
1	D	132	LYS
1	D	134	LEU
1	D	147	THR
1	D	149	MET
1	D	153	ARG
1	D	154	LYS
1	D	156	LEU
1	D	160	LEU
1	D	165	LYS
1	D	166	MET

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Mol	Chain	Res	Type
1	D	168	ASN
1	D	170	GLN
1	D	171	PHE
1	D	172	GLU
1	D	174	LEU
1	D	175	VAL
1	D	177	GLU
1	D	180	ASP
1	D	181	ILE
1	D	182	PHE
1	D	187	ASN
1	D	217	THR
1	D	228	LEU
1	D	243	GLU
1	D	251	ASN
1	D	252	ARG
1	D	253	GLU
1	D	258	MET
1	D	263	LEU
1	D	268	ILE
1	D	270	LYS
1	D	272	ASP
1	D	273	SER
1	D	278	LEU
1	D	295	PRO
1	D	307	LEU
1	D	308	LEU
1	D	317	ARG
1	D	327	LEU
1	D	332	LEU
1	D	343	ASP
1	D	344	LEU
1	D	352	ASP
1	D	354	LYS
1	D	356	THR
1	D	364	LEU
1	D	405	GLN
1	D	409	GLU
1	E	3	VAL
1	E	11	ASN
1	E	31	TYR
1	E	35	SER

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Mol	Chain	Res	Type
1	E	40	LEU
1	E	42	ILE
1	E	46	LYS
1	E	49	SER
1	E	55	VAL
1	E	57	GLN
1	E	60	LYS
1	E	67	ILE
1	E	74	TYR
1	E	94	ASN
1	E	97	LYS
1	E	100	ASP
1	E	101	THR
1	E	108	VAL
1	E	117	LEU
1	E	121	VAL
1	E	126	ARG
1	E	131	ASP
1	E	132	LYS
1	E	134	LEU
1	E	147	THR
1	E	149	MET
1	E	153	ARG
1	E	154	LYS
1	E	156	LEU
1	E	160	LEU
1	E	165	LYS
1	E	166	MET
1	E	167	ILE
1	E	170	GLN
1	E	171	PHE
1	E	172	GLU
1	E	174	LEU
1	E	177	GLU
1	E	180	ASP
1	E	181	ILE
1	E	182	PHE
1	E	187	ASN
1	E	217	THR
1	E	228	LEU
1	E	243	GLU
1	E	251	ASN

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Mol	Chain	Res	Type
1	E	252	ARG
1	E	253	GLU
1	E	258	MET
1	E	263	LEU
1	E	268	ILE
1	E	270	LYS
1	E	272	ASP
1	E	273	SER
1	E	307	LEU
1	E	308	LEU
1	E	317	ARG
1	E	327	LEU
1	E	332	LEU
1	E	343	ASP
1	E	352	ASP
1	E	354	LYS
1	E	356	THR
1	E	359	ASP
1	E	360	SER
1	E	365	THR
1	E	379	LEU
1	E	385	GLN
1	E	405	GLN
1	E	409	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	57	GLN
1	A	70	ASN
1	A	162	ASN
1	A	190	ASN
1	A	266	GLN
1	A	302	GLN
1	A	347	GLN
1	A	395	GLN
1	B	11	ASN
1	B	57	GLN
1	B	70	ASN
1	B	162	ASN
1	B	190	ASN

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Mol	Chain	Res	Type
1	B	266	GLN
1	B	302	GLN
1	B	347	GLN
1	B	395	GLN
1	C	11	ASN
1	C	57	GLN
1	C	70	ASN
1	C	170	GLN
1	C	190	ASN
1	C	266	GLN
1	C	302	GLN
1	C	347	GLN
1	C	385	GLN
1	C	395	GLN
1	D	11	ASN
1	D	57	GLN
1	D	70	ASN
1	D	162	ASN
1	D	190	ASN
1	D	266	GLN
1	D	302	GLN
1	D	347	GLN
1	D	385	GLN
1	D	395	GLN
1	E	11	ASN
1	E	57	GLN
1	E	70	ASN
1	E	190	ASN
1	E	266	GLN
1	E	302	GLN
1	E	347	GLN
1	E	385	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%)	24 (54%)	3 (6%)

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	2	G
2	R	3	G
2	R	5	G
2	R	8	G
2	R	10	G
2	R	13	G
2	R	14	G
2	R	18	G
2	R	21	G
2	R	22	G
2	R	23	G
2	R	25	G
2	R	26	G
2	R	27	G
2	R	28	G
2	R	30	G
2	R	31	G
2	R	32	G
2	R	36	G
2	R	39	G
2	R	40	G
2	R	41	G
2	R	42	G
2	R	45	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	17	G
2	R	18	G
2	R	26	G

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 20 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	421/421 (100%)	0.21	14 (3%)	46	25	56, 92, 130, 142	0
1	B	415/421 (98%)	0.20	16 (3%)	39	20	57, 91, 130, 141	0
1	C	413/421 (98%)	0.21	16 (3%)	39	20	56, 92, 129, 142	0
1	D	416/421 (98%)	0.31	21 (5%)	28	13	56, 92, 130, 141	0
1	E	421/421 (100%)	0.37	37 (8%)	10	4	57, 93, 131, 147	0
2	R	45/45 (100%)	4.36	43 (95%)	0	0	118, 132, 143, 145	0
All	All	2131/2150 (99%)	0.35	147 (6%)	16	7	56, 93, 131, 147	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	11.5
2	R	18	G	10.4
1	E	2	SER	9.7
1	E	114	ASP	9.7
2	R	37	G	8.8
1	E	362	GLY	8.7
1	B	2	SER	8.5
1	E	363	GLY	8.2
2	R	19	G	8.1
2	R	16	G	8.0
1	A	361	THR	7.7
1	D	113	LEU	7.6
2	R	36	G	7.5
1	D	114	ASP	7.5
1	E	43	ASN	6.9
2	R	45	G	6.6
1	D	43	ASN	6.4
1	C	2	SER	6.1
1	E	118	PRO	6.1

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Mol	Chain	Res	Type	RSRZ
2	R	27	G	6.0
2	R	41	G	6.0
1	E	361	THR	5.9
2	R	14	G	5.8
2	R	10	G	5.7
1	A	362	GLY	5.7
2	R	23	G	5.6
2	R	25	G	5.5
1	E	113	LEU	5.4
1	B	119	ASP	5.3
2	R	40	G	5.3
2	R	1	G	5.2
2	R	43	G	5.1
1	D	119	ASP	5.1
1	D	2	SER	5.0
2	R	28	G	5.0
2	R	9	G	4.8
2	R	17	G	4.8
1	E	364	LEU	4.8
1	A	363	GLY	4.8
1	E	360	SER	4.7
2	R	39	G	4.6
1	D	13	VAL	4.6
1	B	114	ASP	4.6
2	R	32	G	4.3
1	C	357	PRO	4.2
2	R	44	G	4.1
2	R	33	G	4.1
1	C	176	PRO	4.1
2	R	13	G	4.0
1	B	169	GLU	4.0
1	B	112	ALA	3.9
1	E	44	THR	3.9
2	R	20	G	3.8
2	R	3	G	3.8
1	D	166	MET	3.8
1	A	357	PRO	3.7
1	E	117	LEU	3.7
1	E	101	THR	3.7
1	E	89	SER	3.7
2	R	2	G	3.4
2	R	24	G	3.4

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Mol	Chain	Res	Type	RSRZ
2	R	26	G	3.4
2	R	38	G	3.4
1	B	386	ASN	3.4
1	D	112	ALA	3.3
1	A	360	SER	3.1
2	R	4	G	3.1
1	D	6	LYS	3.0
2	R	15	G	3.0
1	E	88	TRP	3.0
1	E	170	GLN	2.9
1	E	112	ALA	2.9
2	R	42	G	2.9
2	R	11	G	2.9
1	C	352	ASP	2.9
1	E	54	TYR	2.9
1	D	371	GLN	2.9
1	D	115	GLY	2.8
1	B	158	ASP	2.8
2	R	31	G	2.8
2	R	5	G	2.8
1	B	118	PRO	2.8
2	R	21	G	2.7
1	C	178	GLY	2.7
1	D	172	GLU	2.7
1	E	115	GLY	2.7
2	R	12	G	2.7
1	B	124	ALA	2.7
1	E	45	THR	2.7
1	E	61	SER	2.6
1	C	89	SER	2.6
1	E	95	ILE	2.6
1	E	171	PHE	2.6
1	A	99	GLY	2.5
2	R	7	G	2.5
2	R	30	G	2.5
1	C	83	LYS	2.5
1	C	215	TYR	2.5
1	D	167	ILE	2.5
1	E	172	GLU	2.5
1	A	364	LEU	2.5
1	E	176	PRO	2.4
2	R	22	G	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	365	THR	2.4
1	A	353	ASN	2.4
1	E	405	GLN	2.4
1	A	177	GLU	2.4
1	B	131	ASP	2.4
1	E	42	ILE	2.4
1	C	346	GLN	2.4
1	A	75	GLY	2.3
1	B	122	SER	2.3
1	D	124	ALA	2.3
1	D	116	VAL	2.3
1	D	56	TYR	2.3
1	E	116	VAL	2.3
1	D	39	PRO	2.3
2	R	29	G	2.2
1	B	346	GLN	2.2
2	R	34	G	2.2
1	A	148	GLN	2.2
1	C	233	HIS	2.2
1	C	99	GLY	2.2
1	E	59	LEU	2.2
1	D	422	LYS	2.2
1	C	122	SER	2.2
1	E	86	LYS	2.2
1	D	165	LYS	2.2
2	R	35	G	2.1
1	B	167	ILE	2.1
1	C	177	GLU	2.1
1	B	173	PRO	2.1
1	A	102	ILE	2.1
1	E	62	GLY	2.1
1	A	367	ASN	2.1
1	C	171	PHE	2.1
1	E	152	TYR	2.1
1	B	366	THR	2.0
1	B	163	GLN	2.0
1	E	73	LEU	2.0
1	D	163	GLN	2.0
1	D	274	TYR	2.0
1	E	149	MET	2.0
1	E	66	ILE	2.0
1	C	14	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	84	LEU	2.0
1	C	62	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IUM	R	538	1/3	0.76	0.10	234,234,234,234	1
3	IUM	R	537	1/3	0.81	0.08	161,161,161,161	1
3	IUM	B	525	1/3	0.81	0.08	157,157,157,157	1
3	IUM	R	536	1/3	0.84	0.14	212,212,212,212	1
3	IUM	A	521	1/3	0.86	0.08	171,171,171,171	1
3	IUM	R	540	1/3	0.87	0.09	238,238,238,238	1
3	IUM	B	527	1/3	0.88	0.07	168,168,168,168	1
3	IUM	D	531	1/3	0.90	0.05	144,144,144,144	1
3	IUM	E	535	1/3	0.91	0.05	160,160,160,160	1
3	IUM	R	539	1/3	0.92	0.11	156,156,156,156	1
3	IUM	A	524	1/3	0.95	0.03	159,159,159,159	1
3	IUM	A	523	1/3	0.95	0.07	177,177,177,177	1
3	IUM	C	530	1/3	0.97	0.04	151,151,151,151	1
3	IUM	C	528	1/3	0.98	0.07	130,130,130,130	1
3	IUM	E	533	1/3	0.98	0.07	152,152,152,152	1
3	IUM	B	526	1/3	0.99	0.15	103,103,103,103	1
3	IUM	A	534	1/3	0.99	0.14	128,128,128,128	0
3	IUM	D	532	1/3	0.99	0.15	119,119,119,119	0
3	IUM	A	522	1/3	0.99	0.15	113,113,113,113	1
3	IUM	C	529	1/3	0.99	0.12	108,108,108,108	1

6.5 Other polymers ⓘ

There are no such residues in this entry.