



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:40 AM UTC

PDB ID : 2PV0 / pdb_00002pv0
Title : DNA methyltransferase 3 like protein (DNMT3L)
Authors : Cheng, X.
Deposited on : 2007-05-09
Resolution : 3.30 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

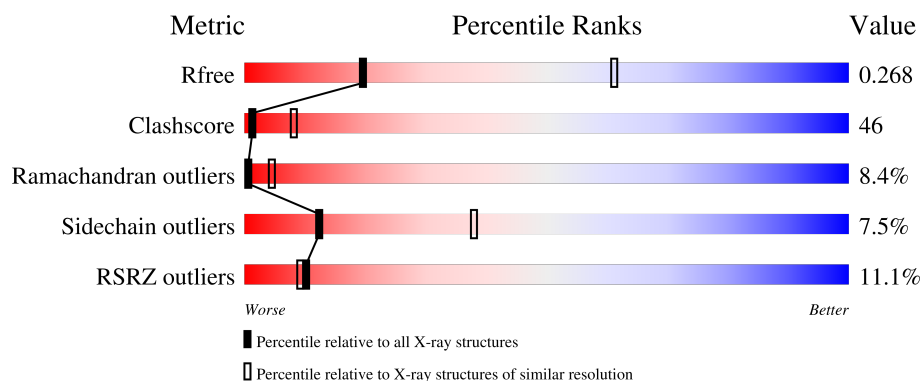
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	4% 37% 42% 11% 10%
1	B	386	4% 33% 47% 10% 10%
1	C	386	23% 36% 43% 10% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7861 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	347	Total	C	N	O	S	0	0	0
			2737	1748	463	505	21			
1	A	347	Total	C	N	O	S	0	0	0
			2744	1753	467	503	21			
1	C	347	Total	C	N	O	S	0	0	0
			2371	1478	415	459	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	278	GLY	ARG	conflict	UNP Q9UJW3
B	?	-	SER	deletion	UNP Q9UJW3
A	278	GLY	ARG	conflict	UNP Q9UJW3
A	?	-	SER	deletion	UNP Q9UJW3
C	278	GLY	ARG	conflict	UNP Q9UJW3
C	?	-	SER	deletion	UNP Q9UJW3

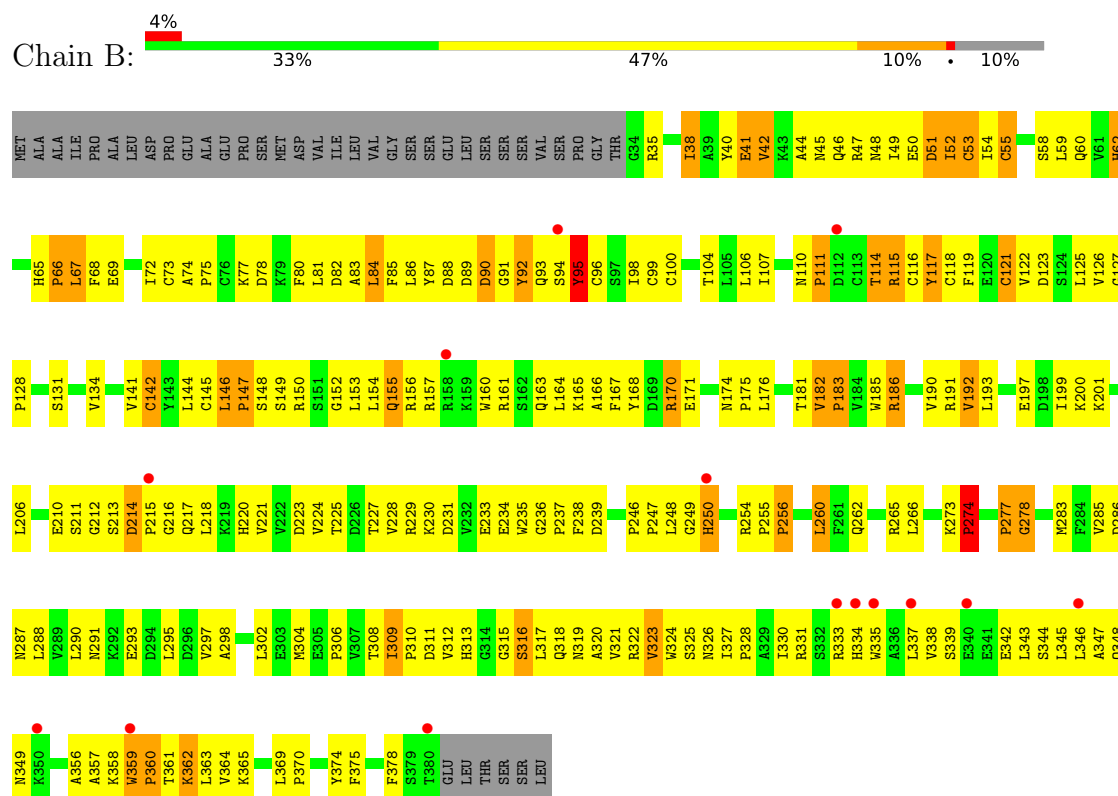
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	3	Total	Zn	0	0
			3	3		
2	C	3	Total	Zn	0	0
			3	3		

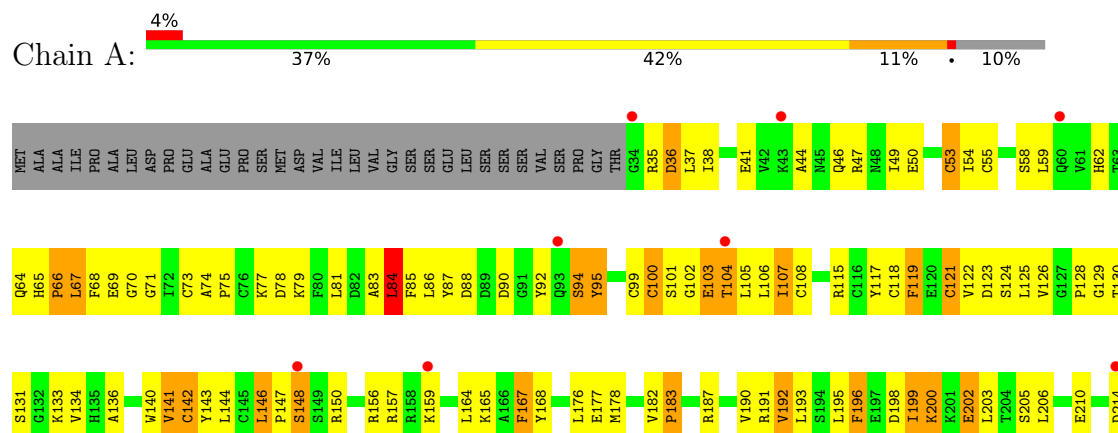
3 Residue-property plots

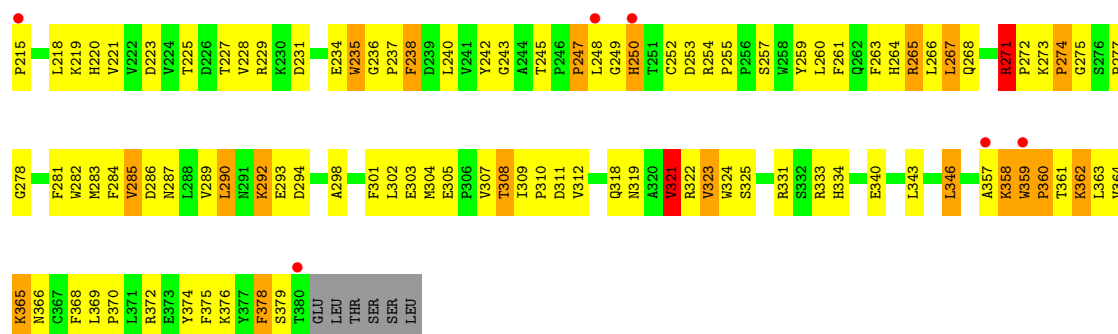
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA (cytosine-5)-methyltransferase 3-like

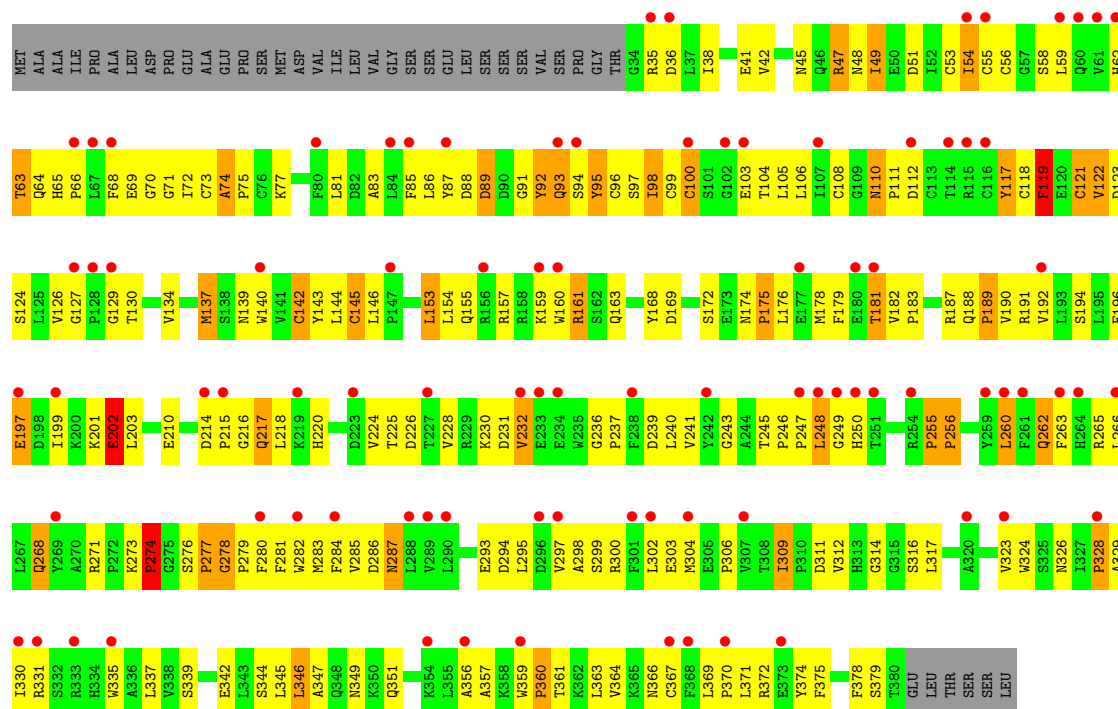


- Molecule 1: DNA (cytosine-5)-methyltransferase 3-like





● Molecule 1: DNA (cytosine-5)-methyltransferase 3-like



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	267.20Å 267.20Å 149.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.74 – 3.30 29.74 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.74-3.30) 98.6 (29.74-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.272 0.243 , 0.268	Depositor DCC
R_{free} test set	2359 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	108.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 109.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7861	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/2821	1.09	21/3840 (0.5%)
1	B	0.48	0/2814	1.10	18/3833 (0.5%)
1	C	0.37	0/2431	0.97	10/3348 (0.3%)
All	All	0.46	0/8066	1.06	49/11021 (0.4%)

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	1

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	VAL	N-CA-C	10.87	120.55	107.61
1	A	359	TRP	CA-C-N	10.47	132.92	119.84
1	A	359	TRP	C-N-CA	10.47	132.92	119.84
1	C	153	LEU	N-CA-C	-9.07	102.22	113.38
1	B	84	LEU	N-CA-C	9.06	121.16	111.28
1	B	67	LEU	N-CA-C	8.47	120.59	111.36
1	C	119	PHE	N-CA-C	-8.40	101.75	112.93
1	A	84	LEU	N-CA-C	8.29	120.40	111.36
1	A	182	VAL	N-CA-C	8.10	117.60	108.05
1	B	330	ILE	N-CA-C	-7.96	104.11	113.42
1	A	119	PHE	N-CA-C	-7.92	100.63	112.04
1	A	67	LEU	N-CA-C	7.78	119.84	111.36
1	B	323	VAL	N-CA-C	7.40	118.98	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	SER	N-CA-C	-7.09	105.17	114.31
1	A	323	VAL	N-CA-C	7.06	117.95	108.27
1	B	359	TRP	CA-C-N	6.76	128.29	119.84
1	B	359	TRP	C-N-CA	6.76	128.29	119.84
1	B	171	GLU	N-CA-C	6.53	120.98	112.89
1	B	192	VAL	N-CA-C	6.44	117.87	108.53
1	B	309	ILE	CA-C-N	6.33	126.51	120.31
1	B	309	ILE	C-N-CA	6.33	126.51	120.31
1	B	182	VAL	CB-CA-C	-6.32	104.00	110.13
1	A	94	SER	N-CA-C	6.15	118.49	111.11
1	B	146	LEU	CA-C-N	5.91	127.22	119.84
1	B	146	LEU	C-N-CA	5.91	127.22	119.84
1	B	95	TYR	N-CA-C	5.72	118.93	110.46
1	A	238	PHE	N-CA-C	5.71	119.03	109.95
1	A	192	VAL	N-CA-C	5.69	117.53	108.89
1	A	271	ARG	CA-C-N	5.67	125.60	119.76
1	A	271	ARG	C-N-CA	5.67	125.60	119.76
1	A	253	ASP	N-CA-C	-5.63	105.52	112.38
1	B	170	ARG	N-CA-C	5.57	117.03	111.07
1	C	137	MET	N-CA-C	5.29	119.66	112.04
1	C	309	ILE	CA-C-N	5.25	125.25	120.21
1	C	309	ILE	C-N-CA	5.25	125.25	120.21
1	A	200	LYS	N-CA-C	5.24	116.67	111.07
1	A	103	GLU	N-CA-C	5.16	117.00	108.48
1	A	285	VAL	N-CA-C	5.16	115.28	107.80
1	B	42	VAL	N-CA-C	5.14	117.48	111.05
1	A	107	ILE	N-CA-C	5.14	116.63	109.80
1	B	35	ARG	N-CA-C	5.09	116.83	111.28
1	C	146	LEU	CA-C-N	5.09	125.12	119.32
1	C	146	LEU	C-N-CA	5.09	125.12	119.32
1	A	255	PRO	CA-C-N	-5.08	113.49	119.84
1	A	255	PRO	C-N-CA	-5.08	113.49	119.84
1	A	275	GLY	N-CA-C	-5.07	108.24	115.64
1	C	331	ARG	N-CA-C	-5.07	107.17	113.55
1	C	105	LEU	N-CA-C	5.06	117.31	108.76
1	C	77	LYS	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2744	0	2625	226	0
1	B	2737	0	2605	247	0
1	C	2371	0	1927	232	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
All	All	7861	0	7157	698	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 (698) 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:A:118:CYS:HB2	1:A:121:CYS:HB2	1.18	1.13
1:B:155:GLN:HA	1:B:155:GLN:HE21	1.17	1.06
1:C:47:ARG:HH11	1:C:47:ARG:HB3	1.15	1.05
1:B:65:HIS:ND1	1:B:72:ILE:HD11	1.72	1.04
1:A:304:MET:HE2	1:A:331:ARG:HH21	1.23	1.03
1:C:118:CYS:HB2	1:C:121:CYS:HB2	1.38	1.03
1:B:144:LEU:HA	1:B:156:ARG:HD3	1.44	1.00
1:C:74:ALA:HB3	1:C:75:PRO:HD3	1.45	0.97
1:B:65:HIS:HD2	1:B:68:PHE:H	1.05	0.97
1:A:118:CYS:CB	1:A:121:CYS:HB2	1.96	0.95
1:B:106:LEU:HD13	1:B:134:VAL:HG11	1.46	0.94
1:A:159:LYS:HE2	1:A:159:LYS:H	1.31	0.94
1:A:83:ALA:HA	1:A:86:LEU:HD12	1.47	0.93
1:A:67:LEU:HD23	1:A:144:LEU:HD11	1.48	0.93
1:C:268:GLN:H	1:C:268:GLN:NE2	1.66	0.93
1:B:122:VAL:O	1:B:126:VAL:HG12	1.68	0.93
1:C:65:HIS:HD2	1:C:68:PHE:H	1.16	0.92
1:B:304:MET:HE2	1:B:331:ARG:HH21	1.33	0.90
1:C:95:TYR:HB3	1:C:100:CYS:HA	1.54	0.90
1:C:281:PHE:HA	1:C:326:ASN:HD21	1.35	0.89
1:C:268:GLN:H	1:C:268:GLN:HE21	1.18	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ALA:HA	1:B:86:LEU:HD23	1.55	0.88
1:A:191:ARG:NH1	1:A:237:PRO:HG2	1.88	0.87
1:C:240:LEU:HA	1:C:281:PHE:O	1.73	0.87
1:B:92:TYR:HD2	1:B:114:THR:HA	1.39	0.86
1:C:312:VAL:HG12	1:C:317:LEU:HA	1.55	0.85
1:B:115:ARG:HD2	1:B:144:LEU:HD12	1.55	0.85
1:B:144:LEU:HA	1:B:156:ARG:CD	2.06	0.85
1:B:285:VAL:HG22	1:B:323:VAL:HG22	1.60	0.84
1:B:155:GLN:HA	1:B:155:GLN:NE2	1.93	0.83
1:A:144:LEU:HA	1:A:156:ARG:HD3	1.60	0.83
1:C:65:HIS:ND1	1:C:72:ILE:HD11	1.94	0.82
1:B:247:PRO:HG3	1:B:359:TRP:HE3	1.43	0.81
1:B:73:CYS:SG	1:B:75:PRO:HD2	2.20	0.81
1:A:118:CYS:HB2	1:A:121:CYS:CB	2.07	0.81
1:A:319:ASN:HA	1:A:346:LEU:HD11	1.63	0.81
1:C:153:LEU:HD23	1:C:153:LEU:O	1.80	0.81
1:C:306:PRO:HG3	1:C:324:TRP:HE1	1.45	0.80
1:B:69:GLU:HB3	1:B:155:GLN:HB3	1.62	0.80
1:C:346:LEU:HD12	1:C:346:LEU:H	1.47	0.79
1:C:278:GLY:H	1:C:279:PRO:HD3	1.45	0.79
1:C:247:PRO:HA	1:C:287:ASN:ND2	1.98	0.79
1:C:54:ILE:O	1:C:54:ILE:HG13	1.83	0.78
1:A:103:GLU:O	1:A:105:LEU:HG	1.82	0.78
1:A:159:LYS:HE2	1:A:159:LYS:N	1.96	0.78
1:C:47:ARG:HB3	1:C:47:ARG:NH1	1.96	0.78
1:A:247:PRO:HA	1:A:287:ASN:HD22	1.47	0.78
1:A:118:CYS:HB3	1:A:121:CYS:H	1.49	0.78
1:C:168:TYR:HD1	1:C:178:MET:SD	2.07	0.78
1:B:65:HIS:CD2	1:B:68:PHE:H	1.96	0.78
1:B:48:ASN:HD22	1:B:50:GLU:HB2	1.49	0.77
1:B:66:PRO:O	1:B:157:ARG:HD2	1.83	0.77
1:C:160:TRP:H	1:C:160:TRP:CD1	2.00	0.77
1:C:53:CYS:HB3	1:C:58:SER:H	1.49	0.76
1:B:92:TYR:CD2	1:B:114:THR:HA	2.21	0.76
1:C:117:TYR:N	1:C:117:TYR:CD1	2.53	0.76
1:B:317:LEU:HD11	1:B:346:LEU:HD21	1.68	0.75
1:B:88:ASP:C	1:B:90:ASP:H	1.94	0.75
1:B:87:TYR:H	1:B:333:ARG:NH2	1.85	0.75
1:B:92:TYR:HB3	1:B:114:THR:O	1.87	0.75
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.66	0.75
1:B:319:ASN:HA	1:B:346:LEU:HD23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:PRO:HG2	1:B:278:GLY:H	1.51	0.74
1:A:67:LEU:HD12	1:A:67:LEU:N	2.01	0.73
1:C:245:THR:HB	1:C:246:PRO:HD2	1.70	0.73
1:B:175:PRO:O	1:B:176:LEU:HD23	1.87	0.73
1:C:53:CYS:SG	1:C:55:CYS:HB3	2.28	0.73
1:A:202:GLU:CD	1:A:202:GLU:H	1.95	0.73
1:B:287:ASN:HB2	1:B:359:TRP:CH2	2.24	0.72
1:C:95:TYR:HB3	1:C:100:CYS:CA	2.19	0.72
1:B:304:MET:HE2	1:B:331:ARG:NH2	2.04	0.72
1:B:47:ARG:HH12	1:B:59:LEU:CD2	2.03	0.72
1:B:106:LEU:HD13	1:B:134:VAL:CG1	2.18	0.72
1:A:193:LEU:HB2	1:A:238:PHE:CE1	2.25	0.72
1:C:83:ALA:HA	1:C:86:LEU:HD23	1.71	0.71
1:B:55:CYS:SG	1:B:99:CYS:HA	2.30	0.71
1:C:95:TYR:HD1	1:C:100:CYS:HB3	1.54	0.71
1:C:260:LEU:HG	1:C:298:ALA:CB	2.21	0.71
1:C:306:PRO:HG3	1:C:324:TRP:NE1	2.05	0.71
1:A:54:ILE:HB	1:A:125:LEU:HD21	1.70	0.71
1:B:287:ASN:HB2	1:B:359:TRP:CZ3	2.26	0.71
1:C:228:VAL:HG22	1:C:231:ASP:OD2	1.90	0.70
1:A:144:LEU:HA	1:A:156:ARG:CD	2.21	0.70
1:A:285:VAL:HG11	1:A:359:TRP:HZ2	1.56	0.70
1:A:118:CYS:O	1:A:122:VAL:HG23	1.92	0.70
1:C:74:ALA:CB	1:C:75:PRO:HD3	2.20	0.70
1:B:155:GLN:HE21	1:B:155:GLN:CA	1.97	0.70
1:C:108:CYS:SG	1:C:110:ASN:HB2	2.32	0.70
1:B:107:ILE:HD13	1:B:116:CYS:CB	2.22	0.69
1:B:328:PRO:HG2	1:B:370:PRO:HB2	1.73	0.69
1:A:53:CYS:SG	1:A:55:CYS:HB2	2.32	0.69
1:C:268:GLN:NE2	1:C:268:GLN:N	2.41	0.69
1:B:164:LEU:O	1:B:167:PHE:HB3	1.92	0.69
1:B:104:THR:HB	1:B:119:PHE:CD1	2.27	0.69
1:C:49:ILE:HG13	1:C:69:GLU:HG2	1.75	0.69
1:C:41:GLU:HA	1:C:45:ASN:OD1	1.92	0.69
1:B:83:ALA:CA	1:B:86:LEU:HD23	2.23	0.68
1:A:308:THR:HG23	1:A:334:HIS:CE1	2.28	0.68
1:A:117:TYR:CE2	1:A:142:CYS:HB2	2.28	0.68
1:A:271:ARG:HG3	1:A:271:ARG:HH11	1.59	0.68
1:B:175:PRO:C	1:B:176:LEU:HD23	2.19	0.68
1:C:276:SER:OG	1:C:277:PRO:HD2	1.95	0.67
1:A:106:LEU:HD13	1:A:134:VAL:HG11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HB2	1:A:147:PRO:HD2	1.76	0.67
1:A:307:VAL:HG21	1:A:331:ARG:HA	1.74	0.67
1:B:95:TYR:N	1:B:95:TYR:HD2	1.91	0.67
1:C:182:VAL:HG23	1:C:374:TYR:HD2	1.58	0.67
1:C:268:GLN:HA	1:C:271:ARG:HG3	1.77	0.67
1:C:122:VAL:HG12	1:C:126:VAL:HG21	1.78	0.66
1:B:88:ASP:O	1:B:90:ASP:N	2.28	0.66
1:A:245:THR:HG21	1:A:290:LEU:HD21	1.77	0.66
1:C:69:GLU:OE2	1:C:155:GLN:HG2	1.95	0.66
1:C:260:LEU:HG	1:C:298:ALA:HB1	1.76	0.66
1:B:191:ARG:NH1	1:B:237:PRO:HG2	2.10	0.66
1:B:260:LEU:C	1:B:260:LEU:HD13	2.21	0.66
1:A:133:LYS:O	1:A:136:ALA:HB3	1.96	0.66
1:B:214:ASP:C	1:B:216:GLY:H	2.02	0.65
1:B:38:ILE:HD11	1:B:125:LEU:HD23	1.79	0.65
1:A:75:PRO:O	1:A:79:LYS:HG2	1.95	0.65
1:C:278:GLY:H	1:C:279:PRO:CD	2.08	0.65
1:B:290:LEU:HB2	1:B:295:LEU:HD13	1.79	0.65
1:C:65:HIS:CD2	1:C:68:PHE:H	2.07	0.65
1:A:35:ARG:O	1:A:38:ILE:HG12	1.96	0.65
1:B:286:ASP:OD2	1:B:290:LEU:HG	1.96	0.65
1:B:325:SER:OG	1:B:327:ILE:HG13	1.96	0.65
1:B:58:SER:OG	1:B:60:GLN:HG2	1.97	0.64
1:B:119:PHE:CD2	1:B:131:SER:HB2	2.32	0.64
1:B:309:ILE:HG13	1:B:309:ILE:O	1.97	0.64
1:A:193:LEU:HB2	1:A:238:PHE:CZ	2.32	0.64
1:C:346:LEU:HD12	1:C:346:LEU:N	2.12	0.64
1:B:107:ILE:HD13	1:B:116:CYS:HB3	1.80	0.64
1:B:306:PRO:HG3	1:B:324:TRP:CE2	2.32	0.64
1:B:317:LEU:HD13	1:B:318:GLN:N	2.12	0.64
1:A:47:ARG:NH1	1:A:59:LEU:HD23	2.12	0.64
1:B:234:GLU:O	1:B:236:GLY:N	2.30	0.64
1:B:248:LEU:HD21	1:B:288:LEU:O	1.97	0.64
1:B:309:ILE:HD11	1:B:363:LEU:HB3	1.80	0.64
1:B:214:ASP:C	1:B:216:GLY:N	2.54	0.64
1:A:242:TYR:CD2	1:A:243:GLY:N	2.66	0.64
1:B:262:GLN:HE22	1:B:265:ARG:NH1	1.96	0.63
1:C:311:ASP:HB2	1:C:363:LEU:HD11	1.78	0.63
1:B:317:LEU:HD22	1:B:318:GLN:H	1.62	0.63
1:A:66:PRO:HB2	1:A:67:LEU:HD12	1.79	0.63
1:B:83:ALA:HA	1:B:86:LEU:CD2	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:GLY:O	1:C:284:PHE:HA	1.99	0.63
1:C:266:LEU:HD12	1:C:266:LEU:H	1.63	0.63
1:A:308:THR:HG23	1:A:334:HIS:HE1	1.63	0.63
1:C:306:PRO:CG	1:C:324:TRP:HE1	2.11	0.63
1:A:104:THR:HB	1:A:119:PHE:H	1.63	0.63
1:C:95:TYR:HD2	1:C:95:TYR:N	1.96	0.63
1:A:190:VAL:HB	1:A:375:PHE:CD1	2.34	0.62
1:B:119:PHE:HD2	1:B:131:SER:HB2	1.63	0.62
1:A:183:PRO:O	1:A:187:ARG:HG3	2.00	0.62
1:B:47:ARG:HH12	1:B:59:LEU:HD23	1.64	0.62
1:B:185:TRP:CD1	1:B:186:ARG:HG3	2.34	0.62
1:C:95:TYR:N	1:C:95:TYR:CD2	2.68	0.62
1:B:123:ASP:HA	1:B:127:GLY:O	2.00	0.61
1:A:286:ASP:HB3	1:A:322:ARG:HB2	1.80	0.61
1:B:92:TYR:HA	1:B:114:THR:HG22	1.82	0.61
1:C:47:ARG:HH11	1:C:47:ARG:CB	2.03	0.61
1:A:304:MET:HE1	1:A:325:SER:O	2.00	0.61
1:B:83:ALA:C	1:B:86:LEU:HD23	2.24	0.61
1:C:281:PHE:HA	1:C:326:ASN:ND2	2.09	0.61
1:C:224:VAL:HG21	1:C:262:GLN:HB3	1.83	0.61
1:B:69:GLU:CB	1:B:155:GLN:HB3	2.30	0.61
1:B:99:CYS:HB3	1:B:121:CYS:SG	2.41	0.61
1:A:193:LEU:HD22	1:A:238:PHE:CE1	2.36	0.61
1:A:146:LEU:HD13	1:A:146:LEU:H	1.66	0.60
1:A:260:LEU:HD21	1:A:302:LEU:HD21	1.83	0.60
1:C:175:PRO:O	1:C:176:LEU:HD23	2.01	0.60
1:A:129:GLY:HA2	1:C:123:ASP:OD2	2.01	0.60
1:A:240:LEU:HA	1:A:281:PHE:O	2.02	0.60
1:B:293:GLU:O	1:B:297:VAL:HG23	2.01	0.60
1:A:115:ARG:CD	1:A:144:LEU:HD12	2.31	0.60
1:B:218:LEU:C	1:B:218:LEU:HD23	2.27	0.60
1:B:122:VAL:C	1:B:126:VAL:HG12	2.26	0.60
1:C:47:ARG:NH1	1:C:51:ASP:HB2	2.16	0.60
1:B:106:LEU:HD22	1:B:134:VAL:HG12	1.83	0.60
1:B:161:ARG:NH1	1:B:181:THR:HB	2.17	0.60
1:A:199:ILE:HG13	1:A:242:TYR:CD1	2.37	0.59
1:A:206:LEU:HD11	1:A:365:LYS:HG3	1.84	0.59
1:A:219:LYS:HE2	1:A:235:TRP:CE2	2.37	0.59
1:B:95:TYR:N	1:B:95:TYR:CD2	2.63	0.59
1:C:293:GLU:C	1:C:295:LEU:H	2.09	0.59
1:B:88:ASP:C	1:B:90:ASP:N	2.60	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLU:O	1:A:47:ARG:HB3	2.03	0.59
1:A:119:PHE:HD2	1:A:131:SER:HB2	1.67	0.59
1:C:47:ARG:HH12	1:C:51:ASP:HB2	1.67	0.59
1:B:304:MET:CE	1:B:331:ARG:HH21	2.13	0.59
1:C:72:ILE:HG22	1:C:73:CYS:N	2.18	0.59
1:B:94:SER:C	1:B:95:TYR:HD2	2.10	0.59
1:C:74:ALA:HB3	1:C:75:PRO:CD	2.25	0.59
1:A:106:LEU:HD22	1:A:134:VAL:HG12	1.84	0.59
1:B:65:HIS:O	1:B:157:ARG:NE	2.33	0.58
1:B:92:TYR:H	1:B:92:TYR:HD1	1.50	0.58
1:B:262:GLN:HE22	1:B:265:ARG:HH12	1.51	0.58
1:C:49:ILE:N	1:C:49:ILE:HD13	2.17	0.58
1:B:247:PRO:HG3	1:B:359:TRP:CE3	2.31	0.58
1:C:130:THR:O	1:C:134:VAL:HG23	2.04	0.58
1:C:224:VAL:HG23	1:C:262:GLN:CD	2.28	0.58
1:C:168:TYR:CD1	1:C:178:MET:SD	2.93	0.58
1:C:94:SER:C	1:C:95:TYR:HD2	2.12	0.57
1:A:50:GLU:OE1	1:A:69:GLU:HG3	2.04	0.57
1:A:248:LEU:N	1:A:248:LEU:HD22	2.19	0.57
1:A:199:ILE:HG22	1:A:203:LEU:HG	1.87	0.57
1:B:117:TYR:N	1:B:117:TYR:CD2	2.72	0.57
1:A:123:ASP:OD2	1:C:129:GLY:HA2	2.05	0.57
1:C:65:HIS:O	1:C:157:ARG:NH1	2.37	0.57
1:B:106:LEU:HD21	1:B:119:PHE:HE2	1.70	0.57
1:C:55:CYS:SG	1:C:99:CYS:HA	2.44	0.57
1:C:181:THR:HG22	1:C:182:VAL:N	2.19	0.57
1:C:181:THR:HG22	1:C:182:VAL:H	1.70	0.57
1:C:49:ILE:HD13	1:C:49:ILE:H	1.69	0.57
1:A:122:VAL:HG12	1:A:130:THR:OG1	2.05	0.56
1:C:49:ILE:HD11	1:C:69:GLU:OE1	2.05	0.56
1:B:168:TYR:CD1	1:B:168:TYR:C	2.83	0.56
1:B:193:LEU:HB2	1:B:238:PHE:CZ	2.40	0.56
1:B:322:ARG:HH11	1:B:322:ARG:HG2	1.70	0.56
1:B:104:THR:HB	1:B:119:PHE:HD1	1.69	0.56
1:B:167:PHE:HA	1:B:170:ARG:HH21	1.70	0.56
1:A:164:LEU:O	1:A:164:LEU:HD23	2.05	0.56
1:C:65:HIS:HB3	1:C:68:PHE:O	2.05	0.56
1:C:69:GLU:HB3	1:C:155:GLN:HB3	1.87	0.56
1:B:328:PRO:HG2	1:B:370:PRO:CB	2.36	0.56
1:A:67:LEU:N	1:A:67:LEU:CD1	2.69	0.56
1:A:357:ALA:O	1:A:358:LYS:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:THR:HG22	1:A:362:LYS:N	2.19	0.56
1:C:72:ILE:HG22	1:C:73:CYS:H	1.71	0.56
1:C:247:PRO:HA	1:C:287:ASN:HD21	1.68	0.56
1:C:284:PHE:O	1:C:324:TRP:HE3	1.89	0.56
1:C:48:ASN:HB3	1:C:51:ASP:OD2	2.06	0.56
1:A:260:LEU:HD21	1:A:302:LEU:CD2	2.35	0.56
1:A:117:TYR:HE2	1:A:142:CYS:HB2	1.70	0.56
1:C:71:GLY:O	1:C:72:ILE:HD13	2.06	0.56
1:B:141:VAL:O	1:B:146:LEU:HD23	2.06	0.56
1:A:191:ARG:HH11	1:A:237:PRO:HG2	1.66	0.56
1:A:99:CYS:O	1:A:100:CYS:HB2	2.06	0.55
1:A:147:PRO:HA	1:A:156:ARG:HH21	1.69	0.55
1:C:346:LEU:H	1:C:346:LEU:CD1	2.16	0.55
1:A:242:TYR:CD2	1:A:242:TYR:C	2.83	0.55
1:A:196:PHE:CD1	1:A:259:TYR:HD2	2.25	0.55
1:C:359:TRP:O	1:C:361:THR:N	2.38	0.55
1:B:95:TYR:HB3	1:B:100:CYS:HA	1.89	0.55
1:B:99:CYS:O	1:B:100:CYS:HB2	2.05	0.55
1:B:214:ASP:N	1:B:215:PRO:HD3	2.21	0.55
1:A:214:ASP:N	1:A:215:PRO:CD	2.70	0.55
1:A:202:GLU:CD	1:A:202:GLU:N	2.65	0.55
1:C:88:ASP:O	1:C:91:GLY:N	2.39	0.55
1:B:152:GLY:O	1:B:153:LEU:HD23	2.07	0.54
1:A:311:ASP:OD1	1:A:318:GLN:HB2	2.07	0.54
1:B:335:TRP:C	1:B:337:LEU:N	2.64	0.54
1:A:77:LYS:HE3	1:A:78:ASP:OD2	2.07	0.54
1:B:74:ALA:HB3	1:B:75:PRO:HD3	1.89	0.54
1:C:314:GLY:C	1:C:316:SER:H	2.16	0.54
1:B:98:ILE:HD13	1:B:154:LEU:HD11	1.90	0.54
1:B:288:LEU:HD11	1:B:320:ALA:HB3	1.90	0.54
1:A:198:ASP:HB2	1:A:220:HIS:CD2	2.43	0.54
1:B:193:LEU:HD22	1:B:238:PHE:CE1	2.42	0.54
1:B:224:VAL:HB	1:B:266:LEU:HD21	1.90	0.54
1:B:230:LYS:O	1:B:234:GLU:HB2	2.08	0.54
1:B:53:CYS:O	1:B:55:CYS:N	2.40	0.54
1:A:260:LEU:HD23	1:A:284:PHE:CE2	2.43	0.54
1:C:110:ASN:OD1	1:C:145:CYS:SG	2.66	0.54
1:B:53:CYS:SG	1:B:55:CYS:HB2	2.48	0.54
1:A:196:PHE:N	1:A:196:PHE:CD2	2.74	0.54
1:A:268:GLN:NE2	1:A:271:ARG:HH12	2.06	0.54
1:C:247:PRO:O	1:C:249:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LEU:HD12	1:B:346:LEU:N	2.23	0.54
1:A:66:PRO:O	1:A:157:ARG:HD2	2.08	0.54
1:A:282:TRP:CZ3	1:A:302:LEU:HD12	2.43	0.54
1:A:307:VAL:CG2	1:A:331:ARG:HA	2.38	0.54
1:C:160:TRP:O	1:C:163:GLN:N	2.41	0.54
1:B:347:ALA:HB3	1:B:348:GLN:OE1	2.08	0.53
1:A:104:THR:O	1:A:118:CYS:HA	2.09	0.53
1:B:81:LEU:HD21	1:B:167:PHE:CE2	2.43	0.53
1:B:322:ARG:HG2	1:B:322:ARG:NH1	2.23	0.53
1:B:356:ALA:C	1:B:358:LYS:H	2.16	0.53
1:B:228:VAL:O	1:B:229:ARG:C	2.51	0.53
1:B:92:TYR:CB	1:B:114:THR:O	2.57	0.53
1:B:359:TRP:HD1	1:B:361:THR:HG23	1.73	0.53
1:B:118:CYS:O	1:B:122:VAL:HG23	2.09	0.53
1:B:190:VAL:HG13	1:B:192:VAL:HG23	1.90	0.53
1:B:291:ASN:O	1:B:295:LEU:HB2	2.09	0.53
1:B:317:LEU:CD1	1:B:346:LEU:HD21	2.39	0.53
1:B:364:VAL:O	1:B:365:LYS:C	2.51	0.53
1:C:49:ILE:CG1	1:C:69:GLU:HG2	2.37	0.53
1:C:96:CYS:C	1:C:98:ILE:H	2.16	0.53
1:C:285:VAL:HA	1:C:323:VAL:HG23	1.90	0.53
1:B:122:VAL:CG1	1:B:126:VAL:HG11	2.39	0.53
1:C:160:TRP:HA	1:C:163:GLN:HB3	1.91	0.53
1:B:360:PRO:HB3	1:B:363:LEU:HD23	1.90	0.52
1:A:94:SER:C	1:A:95:TYR:HD2	2.17	0.52
1:A:290:LEU:N	1:A:290:LEU:HD23	2.24	0.52
1:C:369:LEU:O	1:C:371:LEU:N	2.42	0.52
1:B:92:TYR:N	1:B:92:TYR:CD1	2.77	0.52
1:B:234:GLU:C	1:B:236:GLY:H	2.15	0.52
1:A:54:ILE:HB	1:A:125:LEU:CD2	2.39	0.52
1:A:99:CYS:O	1:A:100:CYS:CB	2.57	0.52
1:C:300:ARG:HA	1:C:300:ARG:CZ	2.40	0.52
1:B:117:TYR:CE2	1:B:142:CYS:HB2	2.45	0.52
1:A:53:CYS:HB2	1:A:73:CYS:H	1.74	0.52
1:C:59:LEU:HD12	1:C:59:LEU:N	2.24	0.52
1:C:83:ALA:CA	1:C:86:LEU:HD23	2.40	0.52
1:B:118:CYS:SG	1:B:121:CYS:HB2	2.50	0.52
1:A:289:VAL:HG22	1:A:289:VAL:O	2.09	0.52
1:B:87:TYR:H	1:B:333:ARG:HH22	1.55	0.52
1:A:168:TYR:CD1	1:A:168:TYR:C	2.88	0.52
1:A:283:MET:HE2	1:A:285:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:MET:HG3	1:A:324:TRP:HD1	1.75	0.52
1:C:225:THR:HG23	1:C:226:ASP:N	2.24	0.52
1:B:304:MET:HE1	1:B:325:SER:O	2.09	0.51
1:A:95:TYR:N	1:A:95:TYR:CD2	2.77	0.51
1:C:99:CYS:O	1:C:100:CYS:HB2	2.09	0.51
1:B:67:LEU:N	1:B:67:LEU:HD23	2.23	0.51
1:A:47:ARG:CZ	1:A:59:LEU:HD23	2.41	0.51
1:A:228:VAL:O	1:A:231:ASP:HB2	2.11	0.51
1:C:68:PHE:CE2	1:C:144:LEU:HD21	2.45	0.51
1:B:122:VAL:HG12	1:B:126:VAL:HG11	1.92	0.51
1:B:325:SER:OG	1:B:326:ASN:N	2.40	0.51
1:A:77:LYS:CE	1:A:78:ASP:OD2	2.59	0.51
1:A:266:LEU:HD12	1:A:266:LEU:H	1.75	0.51
1:A:287:ASN:HA	1:A:321:VAL:HG23	1.92	0.51
1:A:266:LEU:HD12	1:A:266:LEU:N	2.25	0.51
1:C:62:HIS:O	1:C:63:THR:HG23	2.10	0.51
1:C:83:ALA:HA	1:C:86:LEU:CD2	2.40	0.51
1:A:199:ILE:HD11	1:A:242:TYR:CZ	2.46	0.51
1:A:298:ALA:O	1:A:302:LEU:HD23	2.11	0.51
1:C:190:VAL:HG23	1:C:375:PHE:CE2	2.46	0.51
1:B:310:PRO:HB3	1:B:338:VAL:HG21	1.92	0.51
1:A:106:LEU:HD12	1:A:122:VAL:HG21	1.93	0.51
1:C:285:VAL:CA	1:C:323:VAL:HG23	2.41	0.51
1:A:81:LEU:HD23	1:A:167:PHE:HE2	1.75	0.50
1:A:359:TRP:HH2	1:A:364:VAL:HG21	1.76	0.50
1:C:65:HIS:CG	1:C:72:ILE:HD11	2.45	0.50
1:C:108:CYS:C	1:C:110:ASN:H	2.19	0.50
1:C:192:VAL:O	1:C:218:LEU:HA	2.11	0.50
1:A:165:LYS:HE2	1:A:178:MET:O	2.11	0.50
1:A:364:VAL:O	1:A:366:ASN:N	2.44	0.50
1:C:300:ARG:HA	1:C:300:ARG:NE	2.26	0.50
1:B:92:TYR:HB3	1:B:114:THR:CA	2.41	0.50
1:B:277:PRO:HG2	1:B:278:GLY:N	2.23	0.50
1:B:346:LEU:HD12	1:B:346:LEU:H	1.76	0.50
1:C:216:GLY:C	1:C:218:LEU:H	2.20	0.50
1:C:241:VAL:HB	1:C:282:TRP:CB	2.41	0.50
1:C:281:PHE:CE2	1:C:328:PRO:HD3	2.46	0.50
1:B:248:LEU:H	1:B:287:ASN:HD22	1.58	0.50
1:A:264:HIS:ND1	1:A:301:PHE:HD2	2.09	0.50
1:C:65:HIS:CB	1:C:72:ILE:HD11	2.41	0.50
1:A:322:ARG:O	1:A:323:VAL:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:TYR:OH	1:C:142:CYS:HB2	2.12	0.50
1:B:48:ASN:HD22	1:B:50:GLU:CB	2.23	0.50
1:B:66:PRO:HG3	1:B:167:PHE:CG	2.47	0.50
1:A:268:GLN:HE21	1:A:271:ARG:HH12	1.59	0.50
1:A:364:VAL:O	1:A:365:LYS:C	2.54	0.50
1:A:54:ILE:HD13	1:A:70:GLY:HA3	1.92	0.49
1:A:271:ARG:HG3	1:A:271:ARG:NH1	2.27	0.49
1:C:74:ALA:CB	1:C:75:PRO:CD	2.88	0.49
1:A:340:GLU:O	1:A:343:LEU:N	2.45	0.49
1:C:42:VAL:HG11	1:C:153:LEU:HD11	1.93	0.49
1:C:241:VAL:HB	1:C:282:TRP:HA	1.93	0.49
1:B:210:GLU:HB3	1:B:378:PHE:CD1	2.48	0.49
1:B:249:GLY:O	1:B:250:HIS:C	2.54	0.49
1:B:290:LEU:CB	1:B:295:LEU:HD13	2.41	0.49
1:A:115:ARG:NE	1:A:144:LEU:HD12	2.27	0.49
1:C:225:THR:HG23	1:C:226:ASP:H	1.76	0.49
1:A:307:VAL:HG12	1:A:307:VAL:O	2.13	0.49
1:A:198:ASP:C	1:A:200:LYS:H	2.18	0.49
1:C:110:ASN:C	1:C:112:ASP:H	2.21	0.49
1:B:80:PHE:HA	1:B:100:CYS:SG	2.52	0.49
1:A:359:TRP:CD1	1:A:360:PRO:HD2	2.47	0.49
1:B:93:GLN:H	1:B:114:THR:HB	1.78	0.49
1:C:96:CYS:HB3	1:C:100:CYS:H	1.76	0.49
1:C:182:VAL:O	1:C:187:ARG:NH2	2.46	0.49
1:B:51:ASP:OD2	1:B:51:ASP:N	2.45	0.49
1:C:85:PHE:O	1:C:87:TYR:HD1	1.96	0.49
1:C:160:TRP:O	1:C:161:ARG:C	2.56	0.49
1:B:66:PRO:HG3	1:B:167:PHE:CD1	2.48	0.49
1:B:274:PRO:HB3	1:A:274:PRO:HB3	1.94	0.49
1:B:335:TRP:C	1:B:337:LEU:H	2.20	0.49
1:C:183:PRO:O	1:C:187:ARG:HB2	2.12	0.49
1:B:227:THR:O	1:B:265:ARG:NH2	2.46	0.48
1:C:306:PRO:HG3	1:C:324:TRP:CE2	2.47	0.48
1:A:219:LYS:HE2	1:A:235:TRP:CD2	2.48	0.48
1:C:295:LEU:C	1:C:297:VAL:N	2.71	0.48
1:C:306:PRO:HG3	1:C:324:TRP:CZ2	2.48	0.48
1:C:370:PRO:C	1:C:372:ARG:H	2.20	0.48
1:B:346:LEU:H	1:B:346:LEU:CD1	2.27	0.48
1:A:199:ILE:HG22	1:A:199:ILE:O	2.12	0.48
1:A:199:ILE:CG2	1:A:203:LEU:HG	2.44	0.48
1:C:286:ASP:CG	1:C:287:ASN:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:TYR:CD1	1:C:100:CYS:HB3	2.41	0.48
1:C:339:SER:HB3	1:C:342:GLU:CB	2.44	0.48
1:C:369:LEU:C	1:C:371:LEU:N	2.70	0.48
1:B:42:VAL:CG2	1:B:52:ILE:HD11	2.44	0.48
1:A:147:PRO:O	1:A:148:SER:C	2.56	0.48
1:C:201:LYS:C	1:C:203:LEU:H	2.21	0.48
1:C:117:TYR:N	1:C:117:TYR:HD1	2.10	0.48
1:C:190:VAL:HG23	1:C:375:PHE:CD2	2.49	0.48
1:C:344:SER:O	1:C:347:ALA:HB3	2.14	0.48
1:A:268:GLN:HE21	1:A:271:ARG:NH1	2.12	0.48
1:C:268:GLN:HE21	1:C:268:GLN:N	1.98	0.48
1:B:273:LYS:O	1:B:274:PRO:C	2.56	0.48
1:A:44:ALA:O	1:A:46:GLN:HG3	2.14	0.48
1:B:192:VAL:O	1:B:218:LEU:HA	2.14	0.48
1:B:197:GLU:OE2	1:B:197:GLU:HA	2.14	0.48
1:B:220:HIS:HD2	1:B:221:VAL:H	1.61	0.48
1:B:274:PRO:HB3	1:A:274:PRO:CG	2.44	0.48
1:A:210:GLU:N	1:A:378:PHE:CE1	2.82	0.48
1:C:309:ILE:O	1:C:309:ILE:HG13	2.14	0.48
1:B:295:LEU:HD21	1:B:322:ARG:NE	2.29	0.47
1:A:121:CYS:O	1:A:125:LEU:HD12	2.14	0.47
1:A:346:LEU:HD23	1:A:346:LEU:O	2.14	0.47
1:A:369:LEU:N	1:A:370:PRO:CD	2.78	0.47
1:A:363:LEU:N	1:A:363:LEU:HD22	2.29	0.47
1:C:168:TYR:HD1	1:C:178:MET:CE	2.27	0.47
1:B:62:HIS:ND1	1:B:62:HIS:C	2.72	0.47
1:A:199:ILE:HG13	1:A:242:TYR:CE1	2.49	0.47
1:A:218:LEU:HD23	1:A:218:LEU:C	2.38	0.47
1:B:161:ARG:NH1	1:B:161:ARG:HG2	2.28	0.47
1:A:35:ARG:C	1:A:37:LEU:H	2.22	0.47
1:C:224:VAL:HB	1:C:266:LEU:HD11	1.96	0.47
1:C:263:PHE:C	1:C:265:ARG:N	2.71	0.47
1:B:165:LYS:O	1:B:166:ALA:C	2.56	0.47
1:A:199:ILE:O	1:A:199:ILE:CG2	2.61	0.47
1:A:261:PHE:O	1:A:264:HIS:HB3	2.14	0.47
1:C:189:PRO:O	1:C:375:PHE:HD2	1.97	0.47
1:C:228:VAL:HG23	1:C:230:LYS:H	1.79	0.47
1:B:122:VAL:HG12	1:B:126:VAL:CG1	2.45	0.47
1:A:283:MET:HE1	1:A:364:VAL:HB	1.97	0.47
1:A:376:LYS:HD3	1:A:378:PHE:CE2	2.49	0.47
1:C:168:TYR:HD2	1:C:172:SER:HB2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ARG:HG2	1:C:217:GLN:CB	2.45	0.47
1:C:194:SER:OG	1:C:220:HIS:HA	2.14	0.47
1:C:92:TYR:O	1:C:93:GLN:C	2.58	0.47
1:C:295:LEU:C	1:C:297:VAL:H	2.23	0.47
1:B:48:ASN:ND2	1:B:50:GLU:CG	2.77	0.47
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.82	0.47
1:A:247:PRO:HG3	1:A:359:TRP:HD1	1.80	0.47
1:C:284:PHE:O	1:C:324:TRP:CE3	2.68	0.47
1:B:53:CYS:C	1:B:55:CYS:H	2.22	0.47
1:A:81:LEU:HD23	1:A:167:PHE:CE2	2.49	0.47
1:A:234:GLU:C	1:A:236:GLY:H	2.22	0.47
1:A:245:THR:HG21	1:A:290:LEU:CD2	2.41	0.47
1:A:263:PHE:O	1:A:267:LEU:HB2	2.15	0.47
1:A:305:GLU:OE2	1:A:305:GLU:HA	2.15	0.47
1:C:121:CYS:O	1:C:122:VAL:C	2.56	0.47
1:C:126:VAL:HG21	1:C:143:TYR:OH	2.14	0.47
1:B:77:LYS:HD2	1:B:77:LYS:C	2.41	0.46
1:B:92:TYR:HB3	1:B:114:THR:C	2.39	0.46
1:B:216:GLY:C	1:B:218:LEU:H	2.21	0.46
1:B:339:SER:HB3	1:B:342:GLU:HG2	1.97	0.46
1:A:59:LEU:N	1:A:59:LEU:HD12	2.30	0.46
1:A:193:LEU:HD22	1:A:238:PHE:HE1	1.80	0.46
1:C:323:VAL:HG22	1:C:324:TRP:N	2.30	0.46
1:B:99:CYS:O	1:B:100:CYS:CB	2.63	0.46
1:A:273:LYS:O	1:A:274:PRO:C	2.57	0.46
1:C:92:TYR:CD1	1:C:92:TYR:N	2.83	0.46
1:C:117:TYR:HD1	1:C:117:TYR:H	1.62	0.46
1:B:53:CYS:O	1:B:53:CYS:SG	2.72	0.46
1:B:149:SER:C	1:B:155:GLN:HE22	2.23	0.46
1:A:289:VAL:HG13	1:A:290:LEU:HD23	1.98	0.46
1:C:140:TRP:HZ2	1:C:143:TYR:CE2	2.33	0.46
1:C:356:ALA:O	1:C:357:ALA:HB3	2.14	0.46
1:A:47:ARG:NH1	1:A:59:LEU:CD2	2.79	0.46
1:C:349:ASN:C	1:C:351:GLN:H	2.23	0.46
1:B:115:ARG:HD2	1:B:144:LEU:CD1	2.37	0.46
1:B:191:ARG:HB2	1:B:239:ASP:OD1	2.16	0.46
1:B:214:ASP:N	1:B:215:PRO:CD	2.78	0.46
1:B:220:HIS:CD2	1:B:221:VAL:N	2.83	0.46
1:C:169:ASP:HA	1:C:175:PRO:HG3	1.97	0.46
1:C:192:VAL:HG22	1:C:240:LEU:CB	2.45	0.46
1:C:345:LEU:C	1:C:347:ALA:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:PRO:HD2	1:B:335:TRP:CE3	2.50	0.46
1:A:65:HIS:HD2	1:A:68:PHE:H	1.64	0.46
1:A:368:PHE:C	1:A:370:PRO:HD2	2.41	0.46
1:A:85:PHE:O	1:A:87:TYR:HD1	1.98	0.46
1:C:202:GLU:H	1:C:202:GLU:CD	2.24	0.46
1:C:283:MET:HA	1:C:324:TRP:O	2.15	0.46
1:B:200:LYS:HG3	1:B:201:LYS:N	2.31	0.46
1:A:107:ILE:CG2	1:A:108:CYS:N	2.79	0.46
1:A:223:ASP:OD2	1:A:254:ARG:NH2	2.49	0.46
1:C:271:ARG:HG2	1:C:280:PHE:CZ	2.51	0.46
1:B:42:VAL:HG23	1:B:52:ILE:HD11	1.98	0.45
1:B:67:LEU:HD22	1:B:160:TRP:CE3	2.51	0.45
1:B:262:GLN:NE2	1:B:265:ARG:NH1	2.64	0.45
1:A:88:ASP:OD2	1:A:94:SER:HA	2.15	0.45
1:A:95:TYR:HD2	1:A:95:TYR:N	2.13	0.45
1:A:359:TRP:HA	1:A:360:PRO:HD3	1.68	0.45
1:C:364:VAL:HA	1:C:367:CYS:SG	2.56	0.45
1:B:277:PRO:CG	1:B:278:GLY:H	2.19	0.45
1:A:64:GLN:HA	1:A:71:GLY:HA2	1.97	0.45
1:C:260:LEU:HD11	1:C:298:ALA:HA	1.97	0.45
1:B:193:LEU:HB2	1:B:238:PHE:CE1	2.51	0.45
1:B:311:ASP:HB2	1:B:319:ASN:O	2.17	0.45
1:A:107:ILE:O	1:A:140:TRP:HE3	1.99	0.45
1:C:119:PHE:O	1:C:122:VAL:HG23	2.17	0.45
1:C:273:LYS:O	1:C:274:PRO:C	2.59	0.45
1:C:317:LEU:CD2	1:C:346:LEU:HD11	2.46	0.45
1:B:220:HIS:CD2	1:B:221:VAL:H	2.34	0.45
1:B:224:VAL:HG23	1:B:262:GLN:HE21	1.82	0.45
1:B:228:VAL:O	1:B:231:ASP:N	2.41	0.45
1:B:306:PRO:HG3	1:B:324:TRP:CZ2	2.51	0.45
1:A:101:SER:O	1:A:103:GLU:N	2.50	0.45
1:A:147:PRO:O	1:A:148:SER:O	2.35	0.45
1:A:219:LYS:HE3	1:A:221:VAL:CG2	2.46	0.45
1:B:53:CYS:C	1:B:55:CYS:N	2.74	0.45
1:B:181:THR:HA	1:B:374:TYR:CE2	2.52	0.45
1:A:150:ARG:HE	1:A:150:ARG:HA	1.82	0.45
1:C:88:ASP:O	1:C:89:ASP:C	2.60	0.45
1:C:364:VAL:C	1:C:366:ASN:N	2.75	0.45
1:B:40:TYR:O	1:B:41:GLU:C	2.59	0.45
1:B:96:CYS:HB3	1:B:100:CYS:H	1.81	0.45
1:B:229:ARG:NH1	1:A:303:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:PRO:HD2	1:B:335:TRP:HE3	1.82	0.45
1:A:249:GLY:O	1:A:250:HIS:C	2.60	0.45
1:C:278:GLY:N	1:C:279:PRO:HD3	2.23	0.45
1:B:150:ARG:N	1:B:155:GLN:HE22	2.15	0.45
1:B:369:LEU:N	1:B:370:PRO:CD	2.80	0.45
1:A:234:GLU:O	1:A:236:GLY:N	2.48	0.45
1:A:331:ARG:C	1:A:333:ARG:H	2.25	0.45
1:C:86:LEU:N	1:C:86:LEU:HD22	2.31	0.45
1:B:369:LEU:N	1:B:370:PRO:HD3	2.32	0.45
1:A:62:HIS:HB2	1:A:74:ALA:N	2.32	0.45
1:A:192:VAL:HG12	1:A:193:LEU:N	2.32	0.45
1:C:188:GLN:O	1:C:189:PRO:O	2.35	0.45
1:C:224:VAL:HG23	1:C:262:GLN:NE2	2.32	0.45
1:B:212:GLY:O	1:B:213:SER:C	2.60	0.44
1:A:104:THR:HB	1:A:119:PHE:N	2.31	0.44
1:A:192:VAL:HG21	1:A:203:LEU:HD13	1.99	0.44
1:C:328:PRO:O	1:C:330:ILE:HG23	2.16	0.44
1:B:312:VAL:HG12	1:B:313:HIS:N	2.32	0.44
1:A:47:ARG:HH12	1:A:59:LEU:CD2	2.30	0.44
1:C:56:CYS:SG	1:C:58:SER:HB2	2.57	0.44
1:C:134:VAL:HA	1:C:137:MET:CE	2.47	0.44
1:A:202:GLU:O	1:A:205:SER:N	2.50	0.44
1:C:110:ASN:O	1:C:112:ASP:N	2.50	0.44
1:C:179:PHE:CD2	1:C:278:GLY:HA3	2.52	0.44
1:A:53:CYS:HB2	1:A:73:CYS:N	2.33	0.44
1:C:49:ILE:HB	1:C:54:ILE:HG21	1.99	0.44
1:C:65:HIS:ND1	1:C:72:ILE:CD1	2.74	0.44
1:A:64:GLN:HB2	1:A:157:ARG:HH21	1.82	0.44
1:C:317:LEU:HG	1:C:346:LEU:HD21	1.97	0.44
1:A:257:SER:HB3	1:A:294:ASP:OD2	2.18	0.44
1:C:35:ARG:O	1:C:124:SER:HB2	2.18	0.44
1:B:147:PRO:O	1:B:148:SER:C	2.59	0.44
1:A:90:ASP:OD1	1:A:92:TYR:HD1	2.00	0.44
1:A:223:ASP:CG	1:A:225:THR:HG22	2.43	0.44
1:B:190:VAL:HG23	1:B:375:PHE:CD1	2.53	0.44
1:B:260:LEU:C	1:B:260:LEU:CD1	2.91	0.44
1:A:35:ARG:O	1:A:37:LEU:N	2.51	0.44
1:A:103:GLU:O	1:A:104:THR:C	2.60	0.44
1:A:176:LEU:O	1:A:177:GLU:C	2.61	0.44
1:B:107:ILE:HA	1:B:116:CYS:HB3	2.00	0.43
1:B:216:GLY:C	1:B:218:LEU:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:THR:H	1:B:334:HIS:CE1	2.36	0.43
1:C:293:GLU:C	1:C:295:LEU:N	2.76	0.43
1:C:359:TRP:HA	1:C:360:PRO:HD3	1.90	0.43
1:B:142:CYS:SG	1:B:145:CYS:HB2	2.58	0.43
1:B:362:LYS:HE3	1:B:362:LYS:H	1.84	0.43
1:A:35:ARG:C	1:A:37:LEU:N	2.76	0.43
1:A:362:LYS:HG3	1:A:363:LEU:HD22	1.99	0.43
1:C:174:ASN:O	1:C:175:PRO:O	2.35	0.43
1:B:229:ARG:O	1:B:233:GLU:HG3	2.17	0.43
1:B:339:SER:O	1:B:342:GLU:HB2	2.18	0.43
1:A:105:LEU:HA	1:A:117:TYR:O	2.19	0.43
1:C:260:LEU:HD13	1:C:260:LEU:C	2.42	0.43
1:C:263:PHE:C	1:C:265:ARG:H	2.25	0.43
1:A:286:ASP:OD2	1:A:286:ASP:C	2.59	0.43
1:C:63:THR:HB	1:C:64:GLN:H	1.51	0.43
1:C:255:PRO:HA	1:C:256:PRO:HD3	1.84	0.43
1:B:223:ASP:OD2	1:B:225:THR:HG22	2.18	0.43
1:A:67:LEU:HD12	1:A:67:LEU:H	1.79	0.43
1:C:117:TYR:OH	1:C:142:CYS:SG	2.77	0.43
1:C:210:GLU:HB3	1:C:378:PHE:CD2	2.53	0.43
1:C:364:VAL:C	1:C:366:ASN:H	2.25	0.43
1:C:369:LEU:C	1:C:371:LEU:H	2.27	0.43
1:B:297:VAL:O	1:B:298:ALA:C	2.62	0.43
1:A:115:ARG:HD3	1:A:144:LEU:HD12	2.00	0.43
1:A:227:THR:HG22	1:A:228:VAL:N	2.34	0.43
1:C:81:LEU:C	1:C:83:ALA:N	2.75	0.43
1:B:45:ASN:N	1:B:45:ASN:HD22	2.16	0.43
1:B:141:VAL:O	1:B:142:CYS:O	2.36	0.43
1:B:206:LEU:HD21	1:B:365:LYS:HE3	2.00	0.43
1:A:361:THR:O	1:A:363:LEU:N	2.51	0.43
1:A:364:VAL:HG23	1:A:365:LYS:N	2.34	0.43
1:C:65:HIS:HA	1:C:66:PRO:HD3	1.88	0.43
1:C:65:HIS:HB2	1:C:72:ILE:HD11	2.01	0.43
1:B:110:ASN:HA	1:B:111:PRO:HD3	1.84	0.43
1:A:147:PRO:HG2	1:A:148:SER:H	1.84	0.43
1:B:318:GLN:HE21	1:B:318:GLN:HA	1.84	0.43
1:A:199:ILE:HG22	1:A:203:LEU:CD1	2.49	0.43
1:C:210:GLU:HG3	1:C:210:GLU:O	2.18	0.43
1:C:245:THR:HB	1:C:246:PRO:CD	2.45	0.43
1:B:210:GLU:HB3	1:B:378:PHE:CE1	2.53	0.43
1:A:248:LEU:N	1:A:248:LEU:CD2	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:THR:OG1	1:C:119:PHE:HB2	2.19	0.43
1:B:81:LEU:CD2	1:B:167:PHE:HE2	2.32	0.42
1:A:141:VAL:O	1:A:146:LEU:HD11	2.19	0.42
1:A:146:LEU:HB2	1:A:147:PRO:CD	2.48	0.42
1:C:86:LEU:CD2	1:C:86:LEU:N	2.83	0.42
1:C:168:TYR:CD2	1:C:172:SER:HB2	2.53	0.42
1:B:45:ASN:N	1:B:45:ASN:ND2	2.67	0.42
1:B:65:HIS:HB3	1:B:68:PHE:O	2.19	0.42
1:B:141:VAL:HG13	1:B:145:CYS:HB3	2.01	0.42
1:B:214:ASP:O	1:B:216:GLY:N	2.52	0.42
1:B:277:PRO:O	1:B:278:GLY:O	2.37	0.42
1:A:67:LEU:CD1	1:A:67:LEU:H	2.32	0.42
1:A:266:LEU:H	1:A:266:LEU:CD1	2.32	0.42
1:A:107:ILE:HG22	1:A:108:CYS:N	2.33	0.42
1:A:128:PRO:HG2	1:C:36:ASP:HB3	2.01	0.42
1:B:182:VAL:O	1:B:183:PRO:C	2.61	0.42
1:C:174:ASN:O	1:C:174:ASN:CG	2.62	0.42
1:C:248:LEU:H	1:C:287:ASN:HD22	1.66	0.42
1:C:262:GLN:CA	1:C:262:GLN:HE21	2.31	0.42
1:B:84:LEU:HD23	1:B:84:LEU:HA	1.83	0.42
1:B:343:LEU:C	1:B:345:LEU:N	2.74	0.42
1:A:369:LEU:O	1:A:372:ARG:HB3	2.19	0.42
1:A:292:LYS:O	1:A:293:GLU:C	2.62	0.42
1:C:65:HIS:HB2	1:C:70:GLY:O	2.20	0.42
1:C:196:PHE:O	1:C:197:GLU:CB	2.67	0.42
1:B:72:ILE:HG22	1:B:73:CYS:O	2.19	0.42
1:B:77:LYS:HD2	1:B:78:ASP:N	2.34	0.42
1:B:85:PHE:CD2	1:B:370:PRO:HB3	2.55	0.42
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.84	0.42
1:C:86:LEU:CD2	1:C:86:LEU:H	2.32	0.42
1:C:370:PRO:C	1:C:372:ARG:N	2.75	0.42
1:B:48:ASN:ND2	1:B:50:GLU:HB2	2.28	0.42
1:A:202:GLU:O	1:A:203:LEU:C	2.63	0.42
1:C:127:GLY:O	1:C:130:THR:HG23	2.19	0.42
1:B:316:SER:O	1:B:317:LEU:HB2	2.20	0.42
1:A:167:PHE:O	1:A:168:TYR:C	2.63	0.42
1:A:319:ASN:CA	1:A:346:LEU:HD11	2.40	0.42
1:A:340:GLU:OE1	1:A:340:GLU:HA	2.20	0.42
1:C:241:VAL:HB	1:C:282:TRP:CA	2.50	0.42
1:A:37:LEU:O	1:A:41:GLU:HG2	2.20	0.42
1:A:311:ASP:HB2	1:A:363:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LEU:H	1:C:287:ASN:ND2	2.18	0.42
1:C:106:LEU:HD12	1:C:118:CYS:O	2.20	0.41
1:C:202:GLU:HB3	1:C:361:THR:HG21	2.01	0.41
1:C:302:LEU:C	1:C:304:MET:H	2.28	0.41
1:B:44:ALA:C	1:B:46:GLN:H	2.28	0.41
1:B:190:VAL:HG23	1:B:375:PHE:CE1	2.54	0.41
1:A:101:SER:HB2	1:A:118:CYS:SG	2.60	0.41
1:A:191:ARG:NH1	1:A:237:PRO:CG	2.74	0.41
1:C:335:TRP:C	1:C:337:LEU:N	2.74	0.41
1:B:347:ALA:C	1:B:349:ASN:H	2.29	0.41
1:C:49:ILE:H	1:C:49:ILE:CD1	2.33	0.41
1:A:53:CYS:HA	1:A:71:GLY:O	2.20	0.41
1:A:84:LEU:HD12	1:A:84:LEU:HA	1.68	0.41
1:A:106:LEU:CD1	1:A:122:VAL:HG21	2.51	0.41
1:A:144:LEU:HD23	1:A:156:ARG:HG3	2.02	0.41
1:A:271:ARG:HA	1:A:272:PRO:HD3	1.83	0.41
1:B:313:HIS:C	1:B:315:GLY:H	2.28	0.41
1:A:368:PHE:C	1:A:370:PRO:CD	2.93	0.41
1:C:45:ASN:HB2	1:C:47:ARG:HG2	2.01	0.41
1:C:122:VAL:HG12	1:C:143:TYR:OH	2.21	0.41
1:C:232:VAL:CG2	1:C:266:LEU:HD23	2.50	0.41
1:B:306:PRO:HG3	1:B:324:TRP:NE1	2.34	0.41
1:C:323:VAL:HG22	1:C:324:TRP:H	1.86	0.41
1:A:292:LYS:NZ	1:A:292:LYS:HB3	2.35	0.41
1:C:161:ARG:HG2	1:C:161:ARG:HH11	1.86	0.41
1:A:220:HIS:ND1	1:A:221:VAL:N	2.68	0.41
1:A:228:VAL:O	1:A:229:ARG:C	2.64	0.41
1:C:199:ILE:O	1:C:199:ILE:HG22	2.21	0.41
1:C:360:PRO:HB3	1:C:363:LEU:HD23	2.03	0.41
1:C:369:LEU:O	1:C:370:PRO:C	2.64	0.41
1:B:199:ILE:O	1:B:199:ILE:HG13	2.19	0.41
1:B:215:PRO:HB2	1:B:217:GLN:NE2	2.36	0.41
1:B:311:ASP:HB3	1:B:318:GLN:HB2	2.03	0.41
1:B:318:GLN:HA	1:B:318:GLN:NE2	2.36	0.41
1:A:38:ILE:HD11	1:A:124:SER:OG	2.21	0.41
1:C:202:GLU:HB3	1:C:361:THR:CG2	2.51	0.41
1:C:300:ARG:HG2	1:C:300:ARG:HH11	1.85	0.41
1:C:328:PRO:O	1:C:330:ILE:N	2.53	0.41
1:B:144:LEU:HA	1:B:156:ARG:HD2	1.98	0.41
1:B:149:SER:OG	1:B:155:GLN:NE2	2.54	0.41
1:B:161:ARG:HG2	1:B:161:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:PRO:HA	1:B:247:PRO:HD3	1.90	0.41
1:B:283:MET:HG3	1:B:325:SER:HB2	2.03	0.41
1:A:260:LEU:CD2	1:A:302:LEU:HD21	2.50	0.41
1:C:53:CYS:C	1:C:55:CYS:H	2.29	0.41
1:C:314:GLY:C	1:C:316:SER:N	2.77	0.41
1:A:157:ARG:HG2	1:A:157:ARG:HH11	1.85	0.40
1:C:96:CYS:C	1:C:98:ILE:N	2.79	0.40
1:C:378:PHE:O	1:C:379:SER:HB3	2.21	0.40
1:B:174:ASN:N	1:B:175:PRO:HD3	2.37	0.40
1:A:195:LEU:C	1:A:196:PHE:CG	2.99	0.40
1:A:260:LEU:C	1:A:260:LEU:HD13	2.46	0.40
1:B:49:ILE:H	1:B:49:ILE:HG13	1.63	0.40
1:B:98:ILE:CD1	1:B:154:LEU:HD11	2.51	0.40
1:B:265:ARG:HD2	1:A:301:PHE:CD1	2.56	0.40
1:A:143:TYR:O	1:A:156:ARG:HD3	2.22	0.40
1:A:146:LEU:HD13	1:A:146:LEU:N	2.33	0.40
1:C:191:ARG:HB2	1:C:239:ASP:OD1	2.21	0.40
1:C:293:GLU:O	1:C:295:LEU:N	2.55	0.40
1:B:346:LEU:N	1:B:346:LEU:CD1	2.85	0.40
1:A:265:ARG:HB3	1:A:266:LEU:HD12	2.03	0.40
1:C:297:VAL:C	1:C:299:SER:N	2.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/386 (89%)	268 (78%)	53 (15%)	24 (7%)	1	7
1	B	345/386 (89%)	254 (74%)	66 (19%)	25 (7%)	1	6
1	C	345/386 (89%)	226 (66%)	81 (24%)	38 (11%)	0	2
All	All	1035/1158 (89%)	748 (72%)	200 (19%)	87 (8%)	0	4

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	ASP
1	B	142	CYS
1	B	147	PRO
1	B	235	TRP
1	B	277	PRO
1	B	278	GLY
1	A	148	SER
1	A	250	HIS
1	C	74	ALA
1	C	103	GLU
1	C	139	ASN
1	C	142	CYS
1	C	189	PRO
1	C	215	PRO
1	C	248	LEU
1	C	277	PRO
1	C	329	ALA
1	B	53	CYS
1	B	91	GLY
1	B	211	SER
1	B	250	HIS
1	B	254	ARG
1	B	316	SER
1	A	36	ASP
1	A	58	SER
1	A	100	CYS
1	A	102	GLY
1	A	199	ILE
1	A	235	TRP
1	A	247	PRO
1	A	278	GLY
1	A	362	LYS
1	A	365	LYS
1	C	159	LYS
1	C	175	PRO
1	C	181	THR
1	C	197	GLU
1	C	255	PRO
1	B	54	ILE
1	B	90	ASP
1	B	115	ARG
1	A	53	CYS

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Mol	Chain	Res	Type
1	A	104	THR
1	A	126	VAL
1	A	142	CYS
1	A	167	PHE
1	A	202	GLU
1	A	358	LYS
1	A	360	PRO
1	C	100	CYS
1	C	111	PRO
1	C	202	GLU
1	C	217	GLN
1	C	237	PRO
1	C	250	HIS
1	C	256	PRO
1	C	294	ASP
1	B	256	PRO
1	B	274	PRO
1	B	344	SER
1	C	89	ASP
1	C	93	GLN
1	C	97	SER
1	C	161	ARG
1	C	303	GLU
1	C	360	PRO
1	B	255	PRO
1	B	357	ALA
1	B	360	PRO
1	A	265	ARG
1	A	277	PRO
1	C	98	ILE
1	C	214	ASP
1	C	274	PRO
1	C	278	GLY
1	C	287	ASN
1	B	41	GLU
1	A	321	VAL
1	B	66	PRO
1	B	214	ASP
1	A	66	PRO
1	B	111	PRO
1	C	38	ILE
1	C	54	ILE

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Mol	Chain	Res	Type
1	C	232	VAL
1	C	328	PRO
1	C	236	GLY

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	301/344 (88%)	279 (93%)	22 (7%)	13	39
1	B	300/344 (87%)	279 (93%)	21 (7%)	14	41
1	C	208/344 (60%)	190 (91%)	18 (9%)	9	32
All	All	809/1032 (78%)	748 (92%)	61 (8%)	12	38

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	ILE
1	B	51	ASP
1	B	52	ILE
1	B	55	CYS
1	B	62	HIS
1	B	82	ASP
1	B	92	TYR
1	B	95	TYR
1	B	114	THR
1	B	117	TYR
1	B	121	CYS
1	B	128	PRO
1	B	155	GLN
1	B	163	GLN
1	B	183	PRO
1	B	186	ARG
1	B	256	PRO
1	B	260	LEU
1	B	274	PRO

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Mol	Chain	Res	Type
1	B	321	VAL
1	B	362	LYS
1	A	36	ASP
1	A	49	ILE
1	A	84	LEU
1	A	95	TYR
1	A	121	CYS
1	A	141	VAL
1	A	146	LEU
1	A	183	PRO
1	A	196	PHE
1	A	252	CYS
1	A	267	LEU
1	A	271	ARG
1	A	274	PRO
1	A	290	LEU
1	A	292	LYS
1	A	308	THR
1	A	309	ILE
1	A	310	PRO
1	A	312	VAL
1	A	321	VAL
1	A	346	LEU
1	A	378	PHE
1	C	47	ARG
1	C	49	ILE
1	C	63	THR
1	C	92	TYR
1	C	95	TYR
1	C	110	ASN
1	C	117	TYR
1	C	119	PHE
1	C	121	CYS
1	C	122	VAL
1	C	145	CYS
1	C	154	LEU
1	C	202	GLU
1	C	260	LEU
1	C	262	GLN
1	C	268	GLN
1	C	274	PRO
1	C	346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	45	ASN
1	B	48	ASN
1	B	60	GLN
1	B	64	GLN
1	B	65	HIS
1	B	93	GLN
1	B	155	GLN
1	B	163	GLN
1	B	217	GLN
1	B	220	HIS
1	B	262	GLN
1	B	287	ASN
1	B	334	HIS
1	B	366	ASN
1	A	65	HIS
1	A	155	GLN
1	A	174	ASN
1	A	264	HIS
1	A	268	GLN
1	A	349	ASN
1	C	48	ASN
1	C	65	HIS
1	C	110	ASN
1	C	262	GLN
1	C	264	HIS
1	C	268	GLN
1	C	287	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	347/386 (89%)	0.16	14 (4%)	42	28	29, 85, 169, 195	0
1	B	347/386 (89%)	0.14	14 (4%)	42	28	32, 81, 191, 200	0
1	C	347/386 (89%)	1.38	88 (25%)	1	1	93, 166, 199, 200	0
All	All	1041/1158 (89%)	0.56	116 (11%)	10	9	29, 112, 195, 200	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	ARG	5.9
1	C	247	PRO	5.2
1	C	93	GLN	4.7
1	C	127	GLY	4.6
1	C	112	ASP	4.6
1	A	215	PRO	4.5
1	B	337	LEU	4.4
1	A	380	THR	4.4
1	C	85	PHE	4.3
1	C	320	ALA	4.3
1	C	87	TYR	4.3
1	C	248	LEU	4.2
1	C	54	ILE	4.1
1	A	104	THR	3.8
1	B	333	ARG	3.8
1	B	250	HIS	3.8
1	B	215	PRO	3.8
1	C	177	GLU	3.8
1	C	238	PHE	3.7
1	C	192	VAL	3.7
1	C	296	ASP	3.7
1	C	367	CYS	3.6
1	A	214	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	250	HIS	3.5
1	C	331	ARG	3.4
1	C	114	THR	3.3
1	A	248	LEU	3.3
1	C	214	ASP	3.3
1	C	264	HIS	3.3
1	B	112	ASP	3.3
1	C	62	HIS	3.3
1	C	251	THR	3.2
1	C	100	CYS	3.2
1	C	68	PHE	3.2
1	C	249	GLY	3.2
1	C	181	THR	3.2
1	C	304	MET	3.1
1	A	60	GLN	3.1
1	C	266	LEU	3.1
1	C	180	GLU	3.1
1	C	67	LEU	3.1
1	C	288	LEU	3.1
1	A	34	GLY	3.1
1	C	356	ALA	3.1
1	C	60	GLN	3.1
1	C	261	PHE	3.1
1	A	250	HIS	3.0
1	C	159	LYS	3.0
1	B	380	THR	3.0
1	A	148	SER	2.9
1	C	280	PHE	2.9
1	A	159	LYS	2.9
1	C	335	TRP	2.9
1	C	199	ILE	2.9
1	C	330	ILE	2.9
1	C	61	VAL	2.8
1	A	357	ALA	2.8
1	C	259	TYR	2.8
1	C	297	VAL	2.8
1	C	289	VAL	2.8
1	A	93	GLN	2.7
1	C	232	VAL	2.7
1	C	284	PHE	2.7
1	C	302	LEU	2.7
1	C	254	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	140	TRP	2.7
1	C	156	ARG	2.6
1	C	66	PRO	2.6
1	C	301	PHE	2.6
1	C	215	PRO	2.6
1	C	80	PHE	2.6
1	C	147	PRO	2.6
1	A	359	TRP	2.6
1	C	263	PHE	2.6
1	C	107	ILE	2.5
1	C	370	PRO	2.5
1	C	307	VAL	2.5
1	B	94	SER	2.5
1	B	340	GLU	2.5
1	A	43	LYS	2.5
1	C	94	SER	2.4
1	B	350	LYS	2.4
1	C	59	LEU	2.4
1	C	368	PHE	2.3
1	B	346	LEU	2.3
1	C	103	GLU	2.3
1	C	328	PRO	2.3
1	C	359	TRP	2.3
1	C	197	GLU	2.3
1	C	128	PRO	2.3
1	C	373	GLU	2.2
1	C	160	TRP	2.2
1	C	333	ARG	2.2
1	C	116	CYS	2.2
1	C	290	LEU	2.2
1	C	102	GLY	2.2
1	C	55	CYS	2.2
1	B	335	TRP	2.2
1	C	227	THR	2.1
1	C	129	GLY	2.1
1	C	223	ASP	2.1
1	C	282	TRP	2.1
1	C	269	TYR	2.1
1	C	260	LEU	2.1
1	C	35	ARG	2.1
1	C	219	LYS	2.1
1	B	158	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	334	HIS	2.1
1	B	359	TRP	2.1
1	C	242	TYR	2.1
1	C	234	GLU	2.1
1	C	323	VAL	2.0
1	C	84	LEU	2.0
1	C	36	ASP	2.0
1	C	233	GLU	2.0
1	C	354	LYS	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 oligosaccharides 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
2	ZN	C	508	1/1	0.97	0.14	104,104,104,104	1
2	ZN	C	509	1/1	0.97	0.06	127,127,127,127	0
2	ZN	C	507	1/1	0.98	0.06	167,167,167,167	1
2	ZN	A	502	1/1	0.99	0.12	48,48,48,48	1
2	ZN	B	505	1/1	0.99	0.10	13,13,13,13	1
2	ZN	A	501	1/1	1.00	0.02	91,91,91,91	1
2	ZN	B	504	1/1	1.00	0.02	59,59,59,59	1
2	ZN	B	506	1/1	1.00	0.04	67,67,67,67	0
2	ZN	A	503	1/1	1.00	0.02	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.