Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 05:12 AM GMT

PDB ID	:	2PV0
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

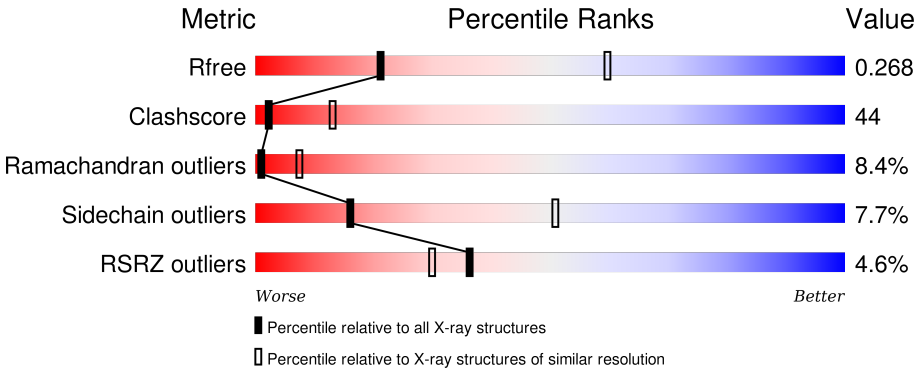
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	386	% 39% 42% 8% 10%
1	B	386	2% 36% 46% 8% 10%
1	C	386	10% 38% 41% 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 (three-letter code: ZN) (formula: Zn).

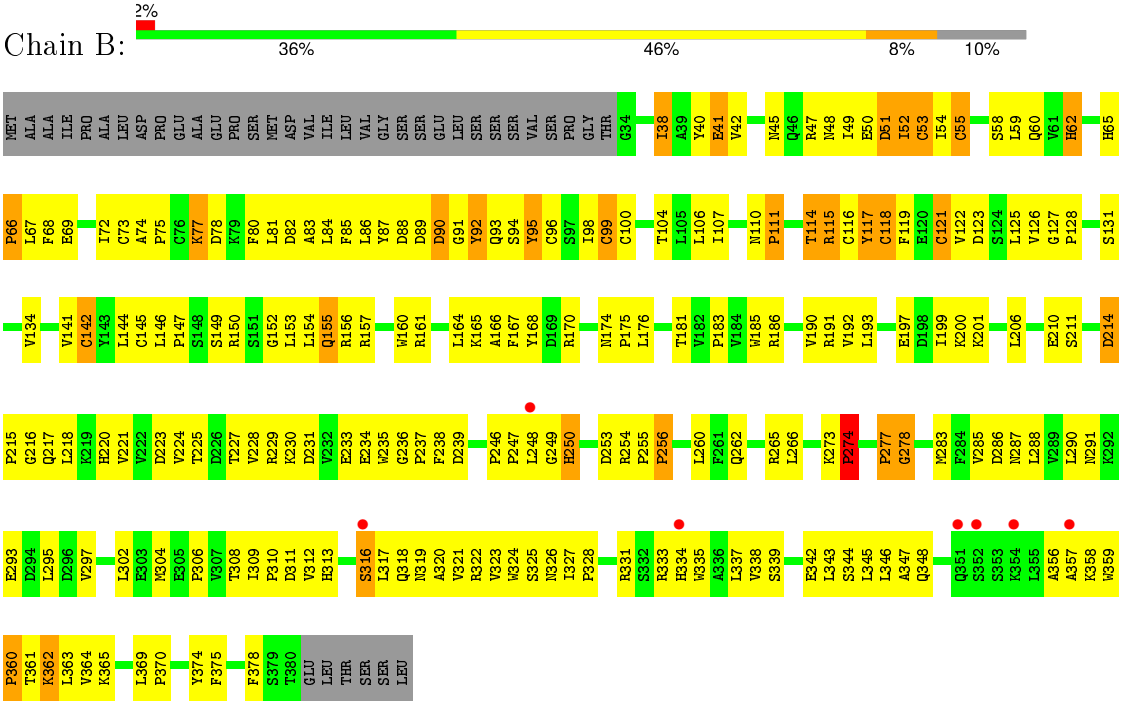
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	3	Total	Zn	0	0
			3	3		
2	C	3	Total	Zn	0	0
			3	3		

3 Residue-property plots (i)

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

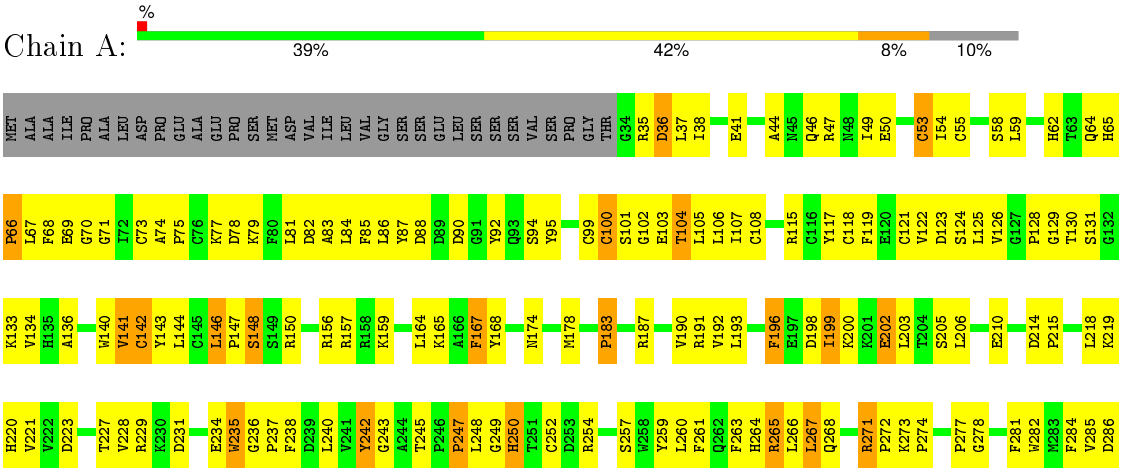
- Molecule 1: DNA (cytosine-5)-methyltransferase 3-like

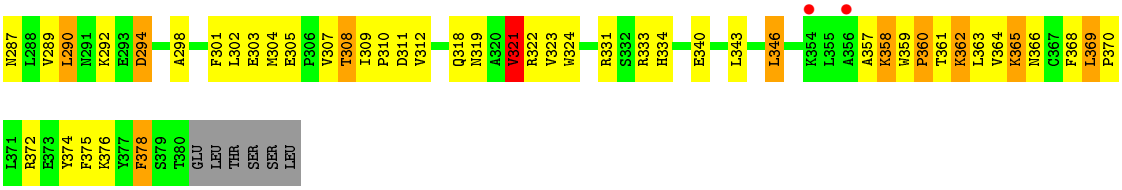
Chain B:



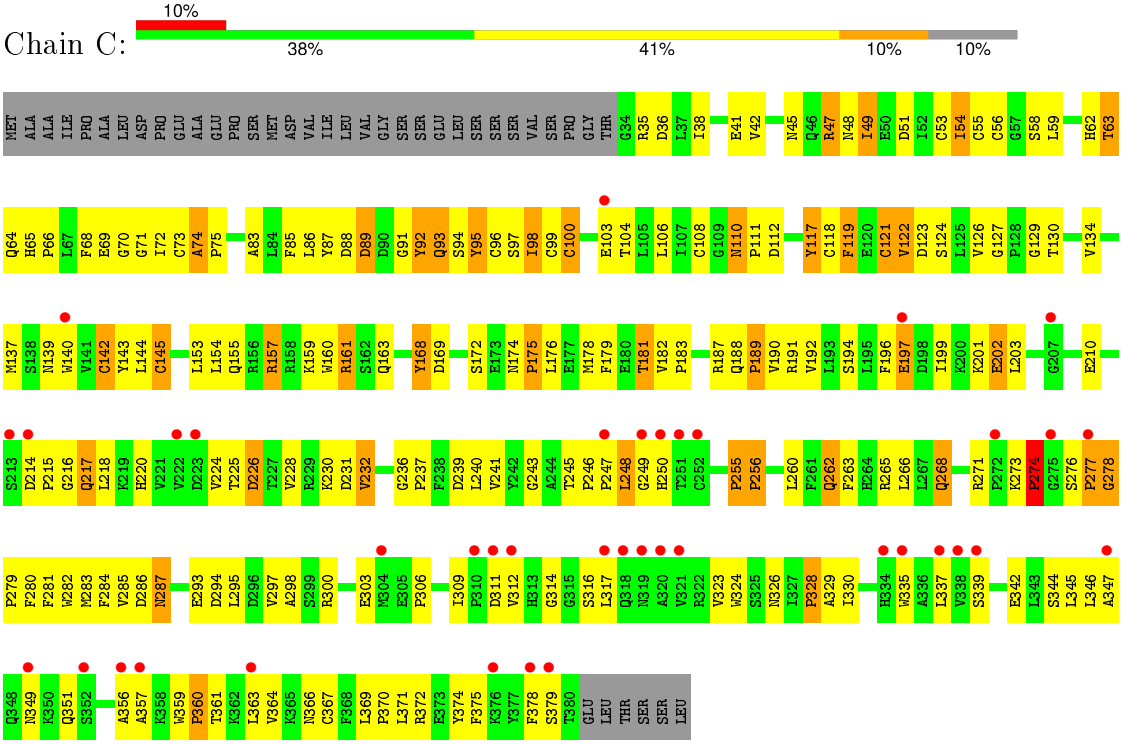
- Molecule 1: DNA (cytosine-5)-methyltransferase 3-like

Chain A:





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



4 Data and refinement statistics (i)

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 34.37 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.74-3.30) 98.8 (34.37-3.29)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	2344 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	108.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 106.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 47265 reflections	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/2821	0.68	1/3840 (0.0%)
1	B	0.42	0/2814	0.69	0/3833
1	C	0.31	0/2431	0.57	0/3348
All	All	0.39	0/8066	0.65	1/11021 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	LEU	CA-CB-CG	-5.19	103.37	115.30

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	212	0
1	B	2737	0	2605	237	0
1	C	2371	0	1927	217	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	659	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 44.

All (659) 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:HB3	1:C:47:ARG:HH11	1.15	1.05
1:B:65:HIS:ND1	1:B:72:ILE:HD11	1.72	1.04
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:C:268:GLN:H	1:C:268:GLN:NE2	1.66	0.93
1:A:67:LEU:HD23	1:A:144:LEU:HD11	1.48	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:153:LEU:O	1:C:153:LEU:HD23	1.80	0.81
1:A:319:ASN:HA	1:A:346:LEU:HD11	1.63	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:N	1:A:159:LYS:HE2	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:66:PRO:O	1:B:157:ARG:HD2	1.83	0.77
1:B:48:ASN:HD22	1:B:50:GLU:HB2	1.49	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: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
1:A:304:MET:HE2	1:A:331:ARG:HH21	1.51	0.74
1:B:277:PRO:HG2	1:B:278:GLY:H	1.51	0.74
1:A:67:LEU:N	1:A:67:LEU:HD12	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:C:95:TYR:HB3	1:C:100:CYS:CA	2.19	0.72
1:B:287:ASN:HB2	1:B:359:TRP:CH2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LEU:HD13	1:B:134:VAL:CG1	2.18	0.72
1:B:47:ARG:HH12	1:B:59:LEU:CD2	2.03	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:306:PRO:HG3	1:C:324:TRP:NE1	2.05	0.71
1:C:260:LEU:HG	1:C:298:ALA:CB	2.21	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:B:88:ASP:C	1:B:90:ASP:H	1.94	0.70
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:CA	1:B:155:GLN:HE21	1.97	0.70
1:C:108:CYS:SG	1:C:110:ASN:HB2	2.32	0.70
1:C:268:GLN:N	1:C:268:GLN:NE2	2.41	0.69
1:A:53:CYS:SG	1:A:55:CYS:HB2	2.32	0.69
1:B:328:PRO:HG2	1:B:370:PRO:HB2	1.73	0.69
1:B:107:ILE:HD13	1:B:116:CYS:CB	2.22	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:202:GLU:CD	1:A:202:GLU:H	1.95	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: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
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:268:GLN:HA	1:C:271:ARG:HG3	1.77	0.67
1:C:182:VAL:HG23	1:C:374:TYR:HD2	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:133:LYS:O	1:A:136:ALA:HB3	1.96	0.66
1:A:75:PRO:O	1:A:79:LYS:HG2	1.95	0.65
1:B:38:ILE:HD11	1:B:125:LEU:HD23	1.79	0.65
1:C:278:GLY:H	1:C:279:PRO:CD	2.08	0.65
1:C:65:HIS:CD2	1:C:68:PHE:H	2.07	0.65
1:B:290:LEU:HB2	1:B:295:LEU:HD13	1.79	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:119:PHE:CD2	1:B:131:SER:HB2	2.32	0.64
1:A:193:LEU:HB2	1:A:238:PHE:CZ	2.32	0.64
1:B:309:ILE:O	1:B:309:ILE:HG13	1.97	0.64
1:B:58:SER:OG	1:B:60:GLN:HG2	1.97	0.64
1:C:346:LEU:HD12	1:C:346:LEU:N	2.12	0.64
1:B:317:LEU:HD13	1:B:318:GLN: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:A:47:ARG:NH1	1:A:59:LEU:HD23	2.12	0.64
1:B:248:LEU:HD21	1:B:288:LEU:O	1.97	0.64
1:B:234:GLU:O	1:B:236:GLY:N	2.30	0.64
1:B:309:ILE:HD11	1:B:363:LEU:HB3	1.80	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
1:C:243:GLY:O	1:C:284:PHE:HA	1.99	0.63
1:C:266:LEU:H	1:C:266:LEU:HD12	1.63	0.63
1:B:175:PRO:C	1:B:176:LEU:HD23	2.19	0.63
1:C:306:PRO:CG	1:C:324:TRP:HE1	2.11	0.63
1:A:308:THR:HG23	1:A:334:HIS:HE1	1.63	0.63
1:A:104:THR:HB	1:A:119:PHE:H	1.63	0.63
1:C:95:TYR:N	1:C:95:TYR:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:214:ASP:C	1:B:216:GLY:H	2.02	0.61
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:C:47:ARG:CB	1:C:47:ARG:HH11	2.03	0.61
1:B:92:TYR:HA	1:B:114:THR:HG22	1.82	0.61
1:B:260:LEU:HD13	1:B:260:LEU:C	2.21	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:H	1:A:146:LEU:HD13	1.66	0.60
1:C:175:PRO:O	1:C:176:LEU:HD23	2.01	0.60
1:A:260:LEU:HD21	1:A:302:LEU:HD21	1.83	0.60
1:A:129:GLY:HA2	1:C:123:ASP:OD2	2.01	0.60
1:B:304:MET:CE	1:B:331:ARG:HH21	2.13	0.60
1:A:240:LEU:HA	1:A:281:PHE:O	2.02	0.60
1:A:115:ARG:CD	1:A:144:LEU:HD12	2.31	0.60
1:B:293:GLU:O	1:B:297:VAL:HG23	2.01	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:206:LEU:HD11	1:A:365:LYS:HG3	1.84	0.59
1:A:199:ILE:HG13	1:A:242:TYR:CD1	2.37	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: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:A:41:GLU:O	1:A:47:ARG:HB3	2.03	0.59
1:C:72:ILE:HG22	1:C:73:CYS:N	2.18	0.59
1:B:304:MET:HE1	1:B:331:ARG:HH21	1.67	0.59
1:C:74:ALA:HB3	1:C:75:PRO:CD	2.25	0.59
1:B:214:ASP:C	1:B:216:GLY:N	2.54	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:HD1	1:B:92:TYR:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:THR:O	1:C:134:VAL:HG23	2.04	0.58
1:C:168:TYR:CD1	1:C:178:MET:SD	2.93	0.58
1:A:50:GLU:OE1	1:A:69:GLU:HG3	2.04	0.57
1:A:248:LEU:HD22	1:A:248:LEU:N	2.19	0.57
1:A:199:ILE:HG22	1:A:203:LEU:HG	1.87	0.57
1:B:117:TYR:CD2	1:B:117:TYR:N	2.72	0.57
1:C:65:HIS:O	1:C:157:ARG:NH1	2.37	0.57
1:A:123:ASP:OD2	1:C:129:GLY:HA2	2.05	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:A:304:MET:CE	1:A:331:ARG:HH21	2.16	0.57
1:C:181:THR:HG22	1:C:182:VAL:H	1.70	0.57
1:C:181:THR:HG22	1:C:182:VAL:N	2.19	0.57
1:C:49:ILE:H	1:C:49:ILE:HD13	1.69	0.57
1:A:122:VAL:HG12	1:A:130:THR:OG1	2.05	0.56
1:B:99:CYS:O	1:B:100:CYS:HB2	2.05	0.56
1:C:49:ILE:HD11	1:C:69:GLU:OE1	2.05	0.56
1:B:322:ARG:HH11	1:B:322:ARG:HG2	1.70	0.56
1:B:193:LEU:HB2	1:B:238:PHE:CZ	2.40	0.56
1:B:167:PHE:HA	1:B:170:ARG:HH21	1.70	0.56
1:B:104:THR:HB	1:B:119:PHE:HD1	1.69	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:A:164:LEU:HD23	1:A:164:LEU:O	2.05	0.56
1:B:83:ALA:C	1:B:86:LEU:HD23	2.24	0.56
1:A:67:LEU:N	1:A:67:LEU:CD1	2.69	0.56
1:C:72:ILE:HG22	1:C:73:CYS:H	1.71	0.56
1:C:284:PHE:O	1:C:324:TRP:HE3	1.89	0.56
1:C:247:PRO:HA	1:C:287:ASN:HD21	1.68	0.56
1:B:328:PRO:HG2	1:B:370:PRO:CB	2.36	0.56
1:A:361:THR:HG22	1:A:362:LYS:N	2.19	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:A:191:ARG:HH11	1:A:237:PRO:HG2	1.66	0.56
1:B:141:VAL:O	1:B:146:LEU:HD23	2.06	0.56
1:A:147:PRO:HA	1:A:156:ARG:HH21	1.69	0.55
1:C:346:LEU:CD1	1:C:346:LEU:H	2.16	0.55
1:A:99:CYS:O	1:A:100:CYS:HB2	2.06	0.55
1:C:359:TRP:O	1:C:361:THR:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LEU:C	1:B:218:LEU:HD23	2.27	0.55
1:A:196:PHE:CD1	1:A:259:TYR:HD2	2.25	0.55
1:B:95:TYR:HB3	1:B:100:CYS:HA	1.89	0.55
1:C:293:GLU:C	1:C:295:LEU:H	2.09	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:B:88:ASP:C	1:B:90:ASP:N	2.60	0.55
1:C:88:ASP:O	1:C:91:GLY:N	2.39	0.55
1:A:311:ASP:OD1	1:A:318:GLN:HB2	2.07	0.54
1:B:152:GLY:O	1:B:153:LEU:HD23	2.07	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:B:94:SER:C	1:B:95:TYR:HD2	2.10	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:98:ILE:HD13	1:B:154:LEU:HD11	1.90	0.54
1:B:230:LYS:O	1:B:234:GLU:HB2	2.08	0.54
1:B:224:VAL:HB	1:B:266:LEU:HD21	1.90	0.54
1:B:193:LEU:HD22	1:B:238:PHE:CE1	2.42	0.54
1:B:122:VAL:C	1:B:126:VAL:HG12	2.26	0.54
1:B:53:CYS:O	1:B:55:CYS:N	2.40	0.54
1:C:110:ASN:OD1	1:C:145:CYS:SG	2.66	0.54
1:A:260:LEU:HD23	1:A:284:PHE:CE2	2.43	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:C:247:PRO:O	1:C:249:GLY:N	2.40	0.54
1:A:268:GLN:NE2	1:A:271:ARG:HH12	2.06	0.54
1:A:66:PRO:O	1:A:157:ARG:HD2	2.08	0.54
1:B:346:LEU:HD12	1:B:346:LEU:N	2.23	0.54
1:A:307:VAL:CG2	1:A:331:ARG:HA	2.38	0.54
1:A:282:TRP:CZ3	1:A:302:LEU:HD12	2.43	0.54
1:C:160:TRP:O	1:C:163:GLN:N	2.41	0.54
1:A:104:THR:O	1:A:118:CYS:HA	2.09	0.53
1:C:224:VAL:HG23	1:C:262:GLN:CD	2.28	0.53
1:B:347:ALA:HB3	1:B:348:GLN:OE1	2.08	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:92:TYR:CB	1:B:114:THR:O	2.57	0.53
1:A:289:VAL:HG22	1:A:289:VAL:O	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:SER:C	1:C:95:TYR:HD2	2.12	0.53
1:C:49:ILE:CG1	1:C:69:GLU:HG2	2.37	0.53
1:B:317:LEU:CD1	1:B:346:LEU:HD21	2.39	0.53
1:B:291:ASN:O	1:B:295:LEU:HB2	2.09	0.53
1:B:190:VAL:HG13	1:B:192:VAL:HG23	1.90	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:290:LEU:HD23	1:A:290:LEU:N	2.24	0.52
1:C:369:LEU:O	1:C:371:LEU:N	2.42	0.52
1:A:54:ILE:HB	1:A:125:LEU:CD2	2.39	0.52
1:C:99:CYS:O	1:C:100:CYS:HB2	2.09	0.52
1:B:92:TYR:N	1:B:92:TYR:CD1	2.77	0.52
1:A:99:CYS:O	1:A:100:CYS:CB	2.57	0.52
1:C:300:ARG:CZ	1:C:300:ARG:HA	2.40	0.52
1:A:53:CYS:HB2	1:A:73:CYS:H	1.74	0.52
1:C:83:ALA:CA	1:C:86:LEU:HD23	2.40	0.52
1:B:117:TYR:CE2	1:B:142:CYS:HB2	2.45	0.52
1:C:59:LEU:N	1:C:59:LEU:HD12	2.24	0.52
1:B:168:TYR:CD1	1:B:168:TYR:C	2.83	0.52
1:B:118:CYS:SG	1:B:121:CYS:HB2	2.50	0.52
1:B:87:TYR:H	1:B:333:ARG:HH22	1.55	0.52
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:325:SER:OG	1:B:326:ASN:N	2.40	0.51
1:A:95:TYR:N	1:A:95:TYR:CD2	2.77	0.51
1:A:357:ALA:O	1:A:358:LYS:C	2.48	0.51
1:A:47:ARG:CZ	1:A:59:LEU:HD23	2.41	0.51
1:B:67:LEU:N	1:B:67:LEU:HD23	2.23	0.51
1:C:68:PHE:CE2	1:C:144:LEU:HD21	2.45	0.51
1:A:228:VAL:O	1:A:231:ASP:HB2	2.11	0.51
1:B:122:VAL:HG12	1:B:126:VAL:HG11	1.92	0.51
1:A:287:ASN:HA	1:A:321:VAL:HG23	1.92	0.51
1:A:77:LYS:CE	1:A:78:ASP:OD2	2.59	0.51
1:A:266:LEU:H	1:A:266:LEU:HD12	1.75	0.51
1:A:242:TYR:CD2	1:A:242:TYR:C	2.83	0.51
1:C:83:ALA:HA	1:C:86:LEU:CD2	2.40	0.51
1:A:266:LEU:N	1:A:266:LEU:HD12	2.25	0.51
1:C:62:HIS:O	1:C:63:THR:HG23	2.10	0.51
1:A:199:ILE:HD11	1:A:242:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:310:PRO:HB3	1:B:338:VAL:HG21	1.92	0.51
1:C:65:HIS:CG	1:C:72:ILE:HD11	2.45	0.50
1:C:192:VAL:O	1:C:218:LEU:HA	2.11	0.50
1:A:359:TRP:HH2	1:A:364:VAL:HG21	1.76	0.50
1:A:81:LEU:HD23	1:A:167:PHE:HE2	1.75	0.50
1:A:364:VAL:O	1:A:366:ASN:N	2.44	0.50
1:C:300:ARG:NE	1:C:300:ARG:HA	2.26	0.50
1:A:165:LYS:HE2	1:A:178:MET:O	2.11	0.50
1:B:92:TYR:HB3	1:B:114:THR:CA	2.41	0.50
1:C:281:PHE:CE2	1:C:328:PRO:HD3	2.46	0.50
1:B:346:LEU:HD12	1:B:346:LEU:H	1.76	0.50
1:B:277:PRO:HG2	1:B:278:GLY:N	2.23	0.50
1:C:241:VAL:HB	1:C:282:TRP:CB	2.41	0.50
1:C:65:HIS:CB	1:C:72:ILE:HD11	2.41	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:117:TYR:OH	1:C:142:CYS:HB2	2.12	0.50
1:A:322:ARG:O	1:A:323:VAL:HG23	2.10	0.50
1:B:335:TRP:C	1:B:337:LEU:N	2.64	0.50
1:B:66:PRO:HG3	1:B:167:PHE:CG	2.47	0.50
1:B:48:ASN:HD22	1:B:50:GLU:CB	2.23	0.50
1:A:268:GLN:HE21	1:A:271:ARG:HH12	1.59	0.50
1:A:54:ILE:HD13	1:A:70:GLY:HA3	1.92	0.49
1:C:74:ALA:CB	1:C:75:PRO:CD	2.88	0.49
1:A:271:ARG:HG3	1:A:271:ARG:NH1	2.27	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:A:340:GLU:O	1:A:343:LEU:N	2.45	0.49
1:A:115:ARG:NE	1:A:144:LEU:HD12	2.27	0.49
1:B:290:LEU:CB	1:B:295:LEU:HD13	2.41	0.49
1:C:225:THR:HG23	1:C:226:ASP:H	1.76	0.49
1:B:210:GLU:HB3	1:B:378:PHE:CD1	2.48	0.49
1:A:307:VAL:HG12	1:A:307:VAL:O	2.13	0.49
1:A:202:GLU:CD	1:A:202:GLU:N	2.65	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:C:96:CYS:HB3	1:C:100:CYS:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLN:H	1:B:114:THR:HB	1.78	0.49
1:C:182:VAL:O	1:C:187:ARG:NH2	2.46	0.49
1:B:51:ASP:N	1:B:51:ASP:OD2	2.45	0.49
1:C:85:PHE:O	1:C:87:TYR:HD1	1.96	0.49
1:B:66:PRO:HG3	1:B:167:PHE:CD1	2.48	0.49
1:C:183:PRO:O	1:C:187:ARG:HB2	2.12	0.49
1:B:274:PRO:HB3	1:A:274:PRO:HB3	1.94	0.49
1:C:306:PRO:HG3	1:C:324:TRP:CE2	2.47	0.48
1:B:227:THR:O	1:B:265:ARG:NH2	2.46	0.48
1:B:356:ALA:C	1:B:358:LYS:H	2.16	0.48
1:C:306:PRO:HG3	1:C:324:TRP:CZ2	2.48	0.48
1:A:219:LYS:HE2	1:A:235:TRP:CD2	2.48	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:B:228:VAL:O	1:B:229:ARG:C	2.51	0.48
1:A:199:ILE:CG2	1:A:203:LEU:HG	2.44	0.48
1:C:314:GLY:C	1:C:316:SER:H	2.16	0.48
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:B:364:VAL:O	1:B:365:LYS:C	2.51	0.48
1:B:42:VAL:CG2	1:B:52:ILE:HD11	2.44	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:C:268:GLN:N	1:C:268:GLN:HE21	1.98	0.48
1:C:96:CYS:C	1:C:98:ILE:H	2.16	0.48
1:A:268:GLN:HE21	1:A:271:ARG:NH1	2.12	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:A:94:SER:C	1:A:95:TYR:HD2	2.17	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:HG13	1:C:309:ILE:O	2.14	0.48
1:B:197:GLU:HA	1:B:197:GLU:OE2	2.14	0.48
1:B:220:HIS:HD2	1:B:221:VAL:H	1.61	0.48
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:B:295:LEU:HD21	1:B:322:ARG:NE	2.29	0.47
1:A:369:LEU:N	1:A:370:PRO:CD	2.78	0.47
1:C:168:TYR:HD1	1:C:178:MET:CE	2.27	0.47
1:A:363:LEU:N	1:A:363:LEU:HD22	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:HG13	1:A:242:TYR:CE1	2.49	0.47
1:B:234:GLU:C	1:B:236:GLY:H	2.15	0.47
1:C:224:VAL:HB	1:C:266:LEU:HD11	1.96	0.47
1:B:161:ARG:NH1	1:B:161:ARG:HG2	2.28	0.47
1:A:199:ILE:CG2	1:A:199:ILE:O	2.61	0.47
1:C:228:VAL:HG23	1:C:230:LYS:H	1.79	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:B:122:VAL:HG12	1:B:126:VAL:CG1	2.45	0.47
1:C:168:TYR:HD2	1:C:172:SER:HB2	1.78	0.47
1:A:376:LYS:HD3	1:A:378:PHE:CE2	2.49	0.47
1:C:194:SER:OG	1:C:220:HIS:HA	2.14	0.47
1:A:168:TYR:CD1	1:A:168:TYR:C	2.88	0.47
1:C:191:ARG:HG2	1:C:217:GLN:CB	2.45	0.47
1:C:284:PHE:O	1:C:324:TRP:CE3	2.68	0.47
1:A:247:PRO:HG3	1:A:359:TRP:HD1	1.80	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:C:126:VAL:HG21	1:C:143:TYR:OH	2.14	0.47
1:A:245:THR:HG21	1:A:290:LEU:CD2	2.41	0.47
1:A:81:LEU:HD23	1:A:167:PHE:CE2	2.49	0.47
1:A:305:GLU:OE2	1:A:305:GLU:HA	2.15	0.47
1:A:263:PHE:O	1:A:267:LEU:HB2	2.15	0.47
1:C:323:VAL:HG22	1:C:324:TRP:N	2.30	0.46
1:A:193:LEU:HD22	1:A:238:PHE:HE1	1.80	0.46
1:A:59:LEU:HD12	1:A:59:LEU:N	2.30	0.46
1:C:356:ALA:O	1:C:357:ALA:HB3	2.14	0.46
1:B:339:SER:HB3	1:B:342:GLU:HG2	1.97	0.46
1:B:99:CYS:O	1:B:100:CYS:CB	2.63	0.46
1:C:117:TYR:HD1	1:C:117:TYR:H	1.62	0.46
1:C:92:TYR:N	1:C:92:TYR:CD1	2.83	0.46
1:C:140:TRP:HZ2	1:C:143:TYR:CE2	2.33	0.46
1:B:53:CYS:SG	1:B:53:CYS:O	2.72	0.46
1:A:289:VAL:HG13	1:A:290:LEU:HD23	1.98	0.46
1:A:47:ARG:NH1	1:A:59:LEU:CD2	2.79	0.46
1:B:115:ARG:HD2	1:B:144:LEU:CD1	2.37	0.46
1:C:192:VAL:HG22	1:C:240:LEU:CB	2.45	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:C:169:ASP:HA	1:C:175:PRO:HG3	1.97	0.46
1:B:220:HIS:CD2	1:B:221:VAL:N	2.83	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:85:PHE:O	1:A:87:TYR:HD1	1.98	0.46
1:C:283:MET:HA	1:C:324:TRP:O	2.15	0.46
1:C:271:ARG:HG2	1:C:280:PHE:CZ	2.51	0.46
1:A:107:ILE:CG2	1:A:108:CYS:N	2.79	0.46
1:B:200:LYS:HG3	1:B:201:LYS:N	2.31	0.46
1:A:223:ASP:OD2	1:A:254:ARG:NH2	2.49	0.46
1:A:359:TRP:HA	1:A:360:PRO:HD3	1.68	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:N	1:A:95:TYR:HD2	2.13	0.45
1:B:67:LEU:HD22	1:B:160:TRP:CE3	2.51	0.45
1:B:42:VAL:HG23	1:B:52:ILE:HD11	1.98	0.45
1:C:364:VAL:HA	1:C:367:CYS:SG	2.56	0.45
1:A:64:GLN:HA	1:A:71:GLY:HA2	1.97	0.45
1:C:216:GLY:C	1:C:218:LEU:H	2.20	0.45
1:B:277:PRO:CG	1:B:278:GLY:H	2.19	0.45
1:C:260:LEU:HD11	1:C:298:ALA:HA	1.97	0.45
1:C:119:PHE:O	1:C:122:VAL:HG23	2.17	0.45
1:C:317:LEU:CD2	1:C:346:LEU:HD11	2.46	0.45
1:B:311:ASP:HB2	1:B:319:ASN:O	2.17	0.45
1:B:193:LEU:HB2	1:B:238:PHE:CE1	2.51	0.45
1:A:107:ILE:O	1:A:140:TRP:HE3	1.99	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:220:HIS:CD2	1:B:221:VAL:H	2.34	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:C:108:CYS:C	1:C:110:ASN:H	2.19	0.45
1:B:306:PRO:HG3	1:B:324:TRP:CZ2	2.51	0.45
1:A:219:LYS:HE3	1:A:221:VAL:CG2	2.46	0.45
1:A:364:VAL:O	1:A:365:LYS:C	2.54	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:B:96:CYS:HB3	1:B:100:CYS:H	1.81	0.45
1:C:278:GLY:N	1:C:279:PRO:HD3	2.23	0.45
1:B:310:PRO:HD2	1:B:335:TRP:HE3	1.82	0.45
1:B:229:ARG:NH1	1:A:303:GLU:OE1	2.50	0.45
1:B:150:ARG:N	1:B:155:GLN:HE22	2.15	0.45
1:C:86:LEU:HD22	1:C:86:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LEU:N	1:B:370:PRO:CD	2.80	0.45
1:A:198:ASP:C	1:A:200:LYS:H	2.18	0.45
1:A:234:GLU:O	1:A:236:GLY:N	2.48	0.45
1:B:249:GLY:O	1:B:250:HIS:C	2.54	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:B:369:LEU:N	1:B:370:PRO:HD3	2.32	0.45
1:C:224:VAL:HG23	1:C:262:GLN:NE2	2.32	0.45
1:C:188:GLN:O	1:C:189:PRO:O	2.35	0.45
1:A:104:THR:HB	1:A:119:PHE:N	2.31	0.44
1:C:328:PRO:O	1:C:330:ILE:HG23	2.16	0.44
1:A:192:VAL:HG21	1:A:203:LEU:HD13	1.99	0.44
1:C:110:ASN:C	1:C:112:ASP:H	2.21	0.44
1:C:56:CYS:SG	1:C:58:SER:HB2	2.57	0.44
1:A:47:ARG:HH12	1:A:59:LEU:CD2	2.30	0.44
1:C:134:VAL:HA	1:C:137:MET:CE	2.47	0.44
1:B:312:VAL:HG12	1:B:313:HIS:N	2.32	0.44
1:C:179:PHE:CD2	1:C:278:GLY:HA3	2.52	0.44
1:C:110:ASN:O	1:C:112:ASP:N	2.50	0.44
1:A:202:GLU:O	1:A:205:SER:N	2.50	0.44
1:A:53:CYS:HB2	1:A:73:CYS:N	2.33	0.44
1:C:65:HIS:ND1	1:C:72:ILE:CD1	2.74	0.44
1:C:49:ILE:HB	1:C:54:ILE:HG21	1.99	0.44
1:C:160:TRP:O	1:C:161:ARG:C	2.56	0.44
1:C:369:LEU:C	1:C:371:LEU:N	2.70	0.44
1:B:335:TRP:C	1:B:337:LEU:H	2.20	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:C:370:PRO:C	1:C:372:ARG:H	2.20	0.44
1:C:35:ARG:O	1:C:124:SER:HB2	2.18	0.44
1:A:257:SER:HB3	1:A:294:ASP:OD2	2.18	0.44
1:C:295:LEU:C	1:C:297:VAL:N	2.71	0.44
1:A:90:ASP:OD1	1:A:92:TYR:HD1	2.00	0.44
1:C:201:LYS:C	1:C:203:LEU:H	2.21	0.44
1:A:147:PRO:O	1:A:148:SER:C	2.56	0.44
1:A:35:ARG:O	1:A:37:LEU:N	2.51	0.44
1:B:190:VAL:HG23	1:B:375:PHE:CD1	2.53	0.44
1:C:286:ASP:CG	1:C:287:ASN:H	2.21	0.43
1:B:107:ILE:HA	1:B:116:CYS:HB3	2.00	0.43
1:C:359:TRP:HA	1:C:360:PRO:HD3	1.90	0.43
1:B:308:THR:H	1:B:334:HIS:CE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ASN:O	1:C:175:PRO:O	2.35	0.43
1:B:142:CYS:SG	1:B:145:CYS:HB2	2.58	0.43
1:A:362:LYS:HG3	1:A:363:LEU:HD22	1.99	0.43
1:B:362:LYS:HE3	1:B:362:LYS:H	1.84	0.43
1:A:105:LEU:HA	1:A:117:TYR:O	2.19	0.43
1:C:121:CYS:O	1:C:122:VAL:C	2.56	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:35:ARG:C	1:A:37:LEU:H	2.22	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: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:B:223:ASP:OD2	1:B:225:THR:HG22	2.18	0.43
1:C:210:GLU:HB3	1:C:378:PHE:CD2	2.53	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:B:273:LYS:O	1:B:274:PRO:C	2.56	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:A:364:VAL:HG23	1:A:365:LYS:N	2.34	0.43
1:B:141:VAL:O	1:B:142:CYS:O	2.36	0.43
1:A:361:THR:O	1:A:363:LEU:N	2.51	0.43
1:B:206:LEU:HD21	1:B:365:LYS:HE3	2.00	0.43
1:B:45:ASN:HD22	1:B:45:ASN:N	2.16	0.43
1:A:147:PRO:HG2	1:A:148:SER:H	1.84	0.43
1:B:110:ASN:HA	1:B:111:PRO:HD3	1.84	0.43
1:B:318:GLN:HE21	1:B:318:GLN:HA	1.84	0.43
1:C:245:THR:HB	1:C:246:PRO:CD	2.45	0.43
1:A:199:ILE:HG22	1:A:203:LEU:CD1	2.49	0.43
1:C:210:GLU:O	1:C:210:GLU:HG3	2.18	0.43
1:C:104:THR:OG1	1:C:119:PHE:HB2	2.19	0.43
1:A:248:LEU:CD2	1:A:248:LEU:N	2.82	0.43
1:B:210:GLU:HB3	1:B:378:PHE:CE1	2.53	0.43
1:B:62:HIS:C	1:B:62:HIS:ND1	2.72	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:168:TYR:CD2	1:C:172:SER:HB2	2.53	0.42
1:C:86:LEU:CD2	1:C:86:LEU:N	2.83	0.42
1:C:263:PHE:C	1:C:265:ARG:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD23	1:A:218:LEU:C	2.38	0.42
1:B:65:HIS:HB3	1:B:68:PHE:O	2.19	0.42
1:A:67:LEU:H	1:A:67:LEU:CD1	2.32	0.42
1:B:277:PRO:O	1:B:278:GLY:O	2.37	0.42
1:B:214:ASP:O	1:B:216:GLY:N	2.52	0.42
1:B:141:VAL:HG13	1:B:145:CYS:HB3	2.01	0.42
1:A:266:LEU:H	1:A:266:LEU:CD1	2.32	0.42
1:B:45:ASN:N	1:B:45:ASN:ND2	2.67	0.42
1:A:107:ILE:HG22	1:A:108:CYS:N	2.33	0.42
1:B:165:LYS:O	1:B:166:ALA:C	2.56	0.42
1:A:128:PRO:HG2	1:C:36:ASP:HB3	2.01	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:C:295:LEU:C	1:C:297:VAL:H	2.23	0.42
1:A:369:LEU:O	1:A:372:ARG:HB3	2.19	0.42
1:B:84:LEU:HA	1:B:84:LEU:HD23	1.83	0.42
1:C:65:HIS:HB2	1:C:70:GLY:O	2.20	0.42
1:C:92:TYR:O	1:C:93:GLN:C	2.58	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:53:CYS:C	1:B:55:CYS:H	2.22	0.42
1:C:86:LEU:H	1:C:86:LEU:CD2	2.32	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:B:77:LYS:HD2	1:B:78:ASP:N	2.34	0.42
1:B:48:ASN:ND2	1:B:50:GLU:HB2	2.28	0.42
1:C:127:GLY:O	1:C:130:THR:HG23	2.19	0.42
1:B:92:TYR:HB3	1:B:114:THR:C	2.39	0.42
1:A:319:ASN:CA	1:A:346:LEU:HD11	2.40	0.42
1:B:316:SER:O	1:B:317:LEU:HB2	2.20	0.42
1:B:216:GLY:C	1:B:218:LEU:H	2.21	0.42
1:C:241:VAL:HB	1:C:282:TRP:CA	2.50	0.42
1:A:340:GLU:HA	1:A:340:GLU:OE1	2.20	0.42
1:A:273:LYS:O	1:A:274:PRO:C	2.57	0.42
1:C:248:LEU:H	1:C:287:ASN:ND2	2.18	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
1:B:149:SER:C	1:B:155:GLN:HE22	2.23	0.41
1:C:106:LEU:HD12	1:C:118:CYS:O	2.20	0.41
1:B:277:PRO:CG	1:B:278:GLY:N	2.81	0.41
1:C:202:GLU:HB3	1:C:361:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:190:VAL:HG23	1:B:375:PHE:CE1	2.54	0.41
1:A:234:GLU:C	1:A:236:GLY:H	2.22	0.41
1:C:349:ASN:C	1:C:351:GLN:H	2.23	0.41
1:B:343:LEU:C	1:B:345:LEU:N	2.74	0.41
1:C:49:ILE:CD1	1:C:49:ILE:H	2.33	0.41
1:C:345:LEU:C	1:C:347:ALA:H	2.23	0.41
1:B:77:LYS:HD2	1:B:77:LYS:C	2.41	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:53:CYS:HA	1:A:71:GLY:O	2.20	0.41
1:A:271:ARG:HA	1:A:272:PRO:HD3	1.83	0.41
1:A:84:LEU:HD12	1:A:84:LEU:HA	1.68	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:A:368:PHE:C	1:A:370:PRO:HD2	2.41	0.41
1:B:53:CYS:C	1:B:55:CYS:N	2.74	0.41
1:C:323:VAL:HG22	1:C:324:TRP:H	1.86	0.41
1:B:306:PRO:HG3	1:B:324:TRP:NE1	2.34	0.41
1:C:202:GLU:H	1:C:202:GLU:CD	2.24	0.41
1:C:161:ARG:HG2	1:C:161:ARG:HH11	1.86	0.41
1:C:335:TRP:C	1:C:337:LEU:N	2.74	0.41
1:A:292:LYS:HB3	1:A:292:LYS:NZ	2.35	0.41
1:C:360:PRO:HB3	1:C:363:LEU:HD23	2.03	0.41
1:A:220:HIS:ND1	1:A:221:VAL:N	2.68	0.41
1:C:199:ILE:O	1:C:199:ILE:HG22	2.21	0.41
1:C:328:PRO:O	1:C:330:ILE:N	2.53	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:B:215:PRO:HB2	1:B:217:GLN:NE2	2.36	0.41
1:C:300:ARG:HH11	1:C:300:ARG:HG2	1.85	0.41
1:B:199:ILE:O	1:B:199:ILE:HG13	2.19	0.41
1:B:149:SER:OG	1:B:155:GLN:NE2	2.54	0.41
1:B:144:LEU:HA	1:B:156:ARG:HD2	1.98	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ARG:HH11	1:B:161:ARG:HG2	1.86	0.41
1:C:273:LYS:O	1:C:274:PRO:C	2.59	0.41
1:A:157:ARG:HH11	1:A:157:ARG:HG2	1.85	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:146:LEU:N	1:A:146:LEU:HD13	2.33	0.40
1:A:143:TYR:O	1:A:156:ARG:HD3	2.22	0.40
1:B:265:ARG:HD2	1:A:301:PHE:CD1	2.56	0.40
1:C:293:GLU:O	1:C:295:LEU:N	2.55	0.40
1:C:88:ASP:O	1:C:89:ASP:C	2.60	0.40
1:B:98:ILE:CD1	1:B:154:LEU:HD11	2.51	0.40
1:C:191:ARG:HB2	1:C:239:ASP:OD1	2.21	0.40
1:C:364:VAL:C	1:C:366:ASN:N	2.75	0.40
1:B:49:ILE:HG13	1:B:49:ILE:H	1.63	0.40
1:B:346:LEU:N	1:B:346:LEU:CD1	2.85	0.40
1:A:331:ARG:C	1:A:333:ARG:H	2.25	0.40
1:A:265:ARG:HB3	1:A:266:LEU:HD12	2.03	0.40
1:B:40:TYR:O	1:B:41:GLU:C	2.59	0.40
1:A:249:GLY:O	1:A:250:HIS:C	2.60	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 11
1	B	345/386 (89%)	254 (74%)	66 (19%)	25 (7%)	1 11
1	C	345/386 (89%)	226 (66%)	81 (24%)	38 (11%)	0 4
All	All	1035/1158 (89%)	748 (72%)	200 (19%)	87 (8%)	1 7

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
1	A	104	THR

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Mol	Chain	Res	Type
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
1	C	232	VAL

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/344 (88%)	279 (93%)	22 (7%)	17	53
1	B	300/344 (87%)	278 (93%)	22 (7%)	17	53
1	C	208/344 (60%)	190 (91%)	18 (9%)	13	45
All	All	809/1032 (78%)	747 (92%)	62 (8%)	16	51

All (62) 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	77	LYS
1	B	82	ASP
1	B	92	TYR
1	B	95	TYR
1	B	99	CYS
1	B	114	THR
1	B	117	TYR
1	B	118	CYS
1	B	121	CYS
1	B	128	PRO
1	B	155	GLN
1	B	183	PRO
1	B	253	ASP
1	B	256	PRO
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	82	ASP
1	A	141	VAL
1	A	146	LEU
1	A	174	ASN
1	A	183	PRO
1	A	196	PHE
1	A	229	ARG
1	A	242	TYR
1	A	252	CYS
1	A	267	LEU
1	A	271	ARG
1	A	290	LEU
1	A	294	ASP
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	157	ARG
1	C	168	TYR
1	C	226	ASP
1	C	262	GLN
1	C	268	GLN
1	C	274	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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	155	GLN
1	B	163	GLN
1	B	217	GLN
1	B	220	HIS
1	B	262	GLN
1	B	287	ASN
1	A	65	HIS
1	A	155	GLN
1	A	174	ASN
1	A	264	HIS
1	A	268	GLN
1	A	287	ASN
1	A	349	ASN
1	C	48	ASN
1	C	64	GLN
1	C	65	HIS
1	C	110	ASN
1	C	135	HIS
1	C	163	GLN
1	C	262	GLN
1	C	264	HIS
1	C	268	GLN
1	C	287	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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 (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	347/386 (89%)	-0.18	2 (0%) 90 88	29, 85, 169, 195	0
1	B	347/386 (89%)	-0.18	7 (2%) 68 62	33, 81, 191, 200	0
1	C	347/386 (89%)	0.41	39 (11%) 7 5	93, 166, 199, 200	0
All	All	1041/1158 (89%)	0.02	48 (4%) 36 30	29, 112, 195, 200	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	ALA	8.4
1	C	250	HIS	5.9
1	C	376	LYS	4.4
1	C	222	VAL	4.4
1	C	311	ASP	3.6
1	C	252	CYS	3.6
1	C	223	ASP	3.5
1	C	357	ALA	3.4
1	C	213	SER	3.3
1	C	251	THR	3.2
1	C	277	PRO	3.2
1	C	214	ASP	3.2
1	C	317	LEU	3.1
1	C	319	ASN	3.1
1	C	310	PRO	3.0
1	B	351	GLN	2.9
1	C	318	GLN	2.9
1	C	249	GLY	2.8
1	C	335	TRP	2.8
1	C	334	HIS	2.8
1	B	316	SER	2.8
1	C	363	LEU	2.7
1	C	304	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	379	SER	2.7
1	C	321	VAL	2.7
1	B	248	LEU	2.7
1	C	207	GLY	2.7
1	C	352	SER	2.6
1	C	338	VAL	2.6
1	B	357	ALA	2.6
1	A	354	LYS	2.6
1	B	334	HIS	2.6
1	C	103	GLU	2.6
1	C	378	PHE	2.5
1	C	356	ALA	2.5
1	C	275	GLY	2.4
1	C	312	VAL	2.4
1	C	140	TRP	2.4
1	C	349	ASN	2.3
1	C	272	PRO	2.3
1	C	337	LEU	2.2
1	C	247	PRO	2.2
1	B	354	LYS	2.2
1	A	356	ALA	2.2
1	C	347	ALA	2.1
1	C	197	GLU	2.0
1	B	352	SER	2.0
1	C	339	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	C	508	1/1	0.87	0.28	1.94	104,104,104,104	1
2	ZN	B	505	1/1	0.98	0.23	0.71	13,13,13,13	1
2	ZN	A	502	1/1	0.97	0.24	0.52	48,48,48,48	1
2	ZN	B	506	1/1	0.98	0.16	-0.11	67,67,67,67	0
2	ZN	A	503	1/1	0.97	0.15	-0.15	75,75,75,75	0
2	ZN	B	504	1/1	0.99	0.13	-0.69	59,59,59,59	1
2	ZN	A	501	1/1	0.98	0.12	-1.04	91,91,91,91	1
2	ZN	C	509	1/1	0.93	0.04	-1.81	127,127,127,127	0
2	ZN	C	507	1/1	0.86	0.03	-2.38	167,167,167,167	1

6.5 Other polymers (i)

There are no such residues in this entry.