



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:35 am BST

PDB ID : 2VYE  
Title : Crystal Structure of the DnaC-ssDNA complex  
Authors : Lo, Y.H.; Tsai, K.L.; Sun, Y.J.; Hsiao, C.D.  
Deposited on : 2008-07-23  
Resolution : 4.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

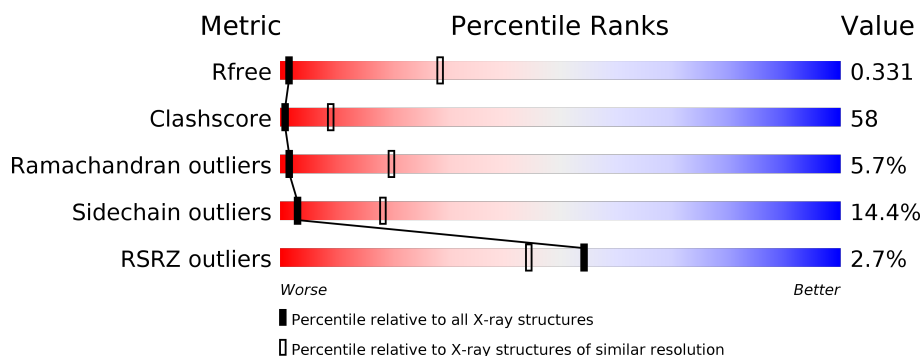
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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  $\geq 3$ , 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	454	<div> <div>2%</div> <div> <div></div> <div>27%</div> <div>54%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	454	<div> <div>3%</div> <div> <div></div> <div>26%</div> <div>46%</div> <div>11%</div> <div>16%</div> </div> </div>
2	C	9	<div> <div>11%</div> <div> <div></div> <div>56%</div> <div>22%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6439 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 REPLICATIVE DNA HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	1
			3310	2058	586	652	14			
1	B	381	Total	C	N	O	S	0	0	1
			2952	1832	526	582	12			

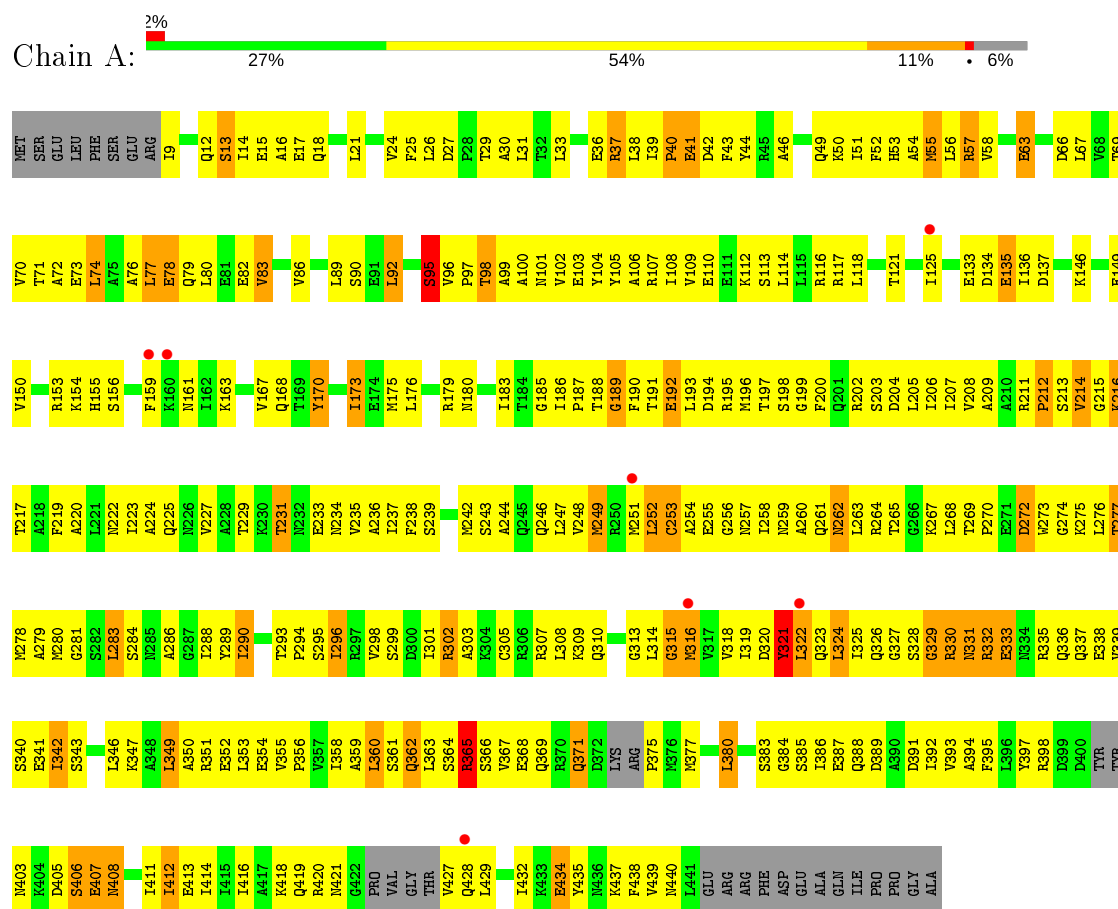
- Molecule 2 is a DNA chain called 5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			177	90	18	61	8			

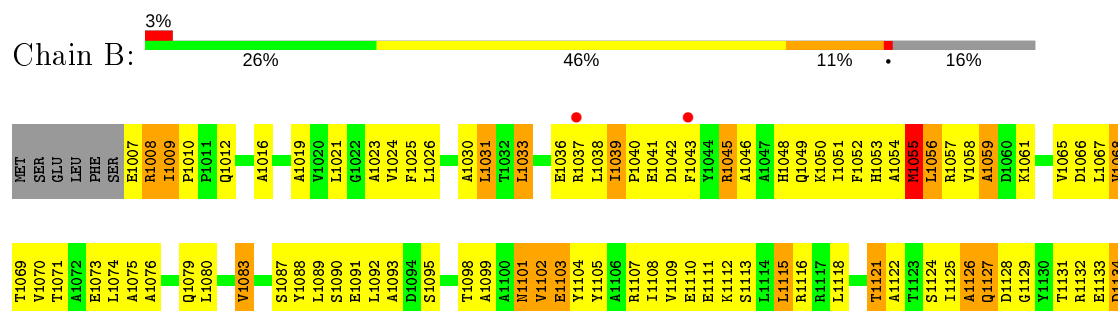
### 3 Residue-property plots

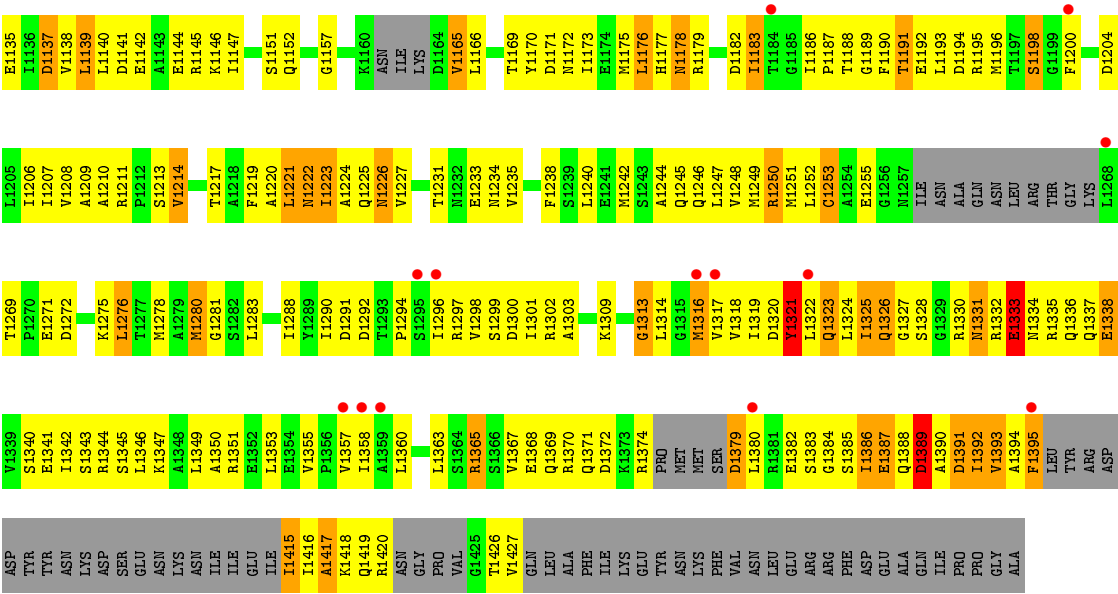
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: REPLICATIVE DNA HELICASE

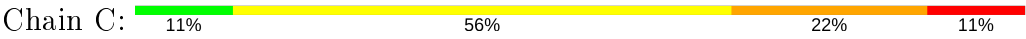


#### • Molecule 1: REPLICATIVE DNA HELICASE





● Molecule 2: 5'-D(\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.83Å 180.83Å 104.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.94 – 4.10 29.94 – 4.09	Depositor EDS
% Data completeness (in resolution range)	76.4 (29.94-4.10) 85.5 (29.94-4.09)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.30 (at 4.11Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.302 , 0.374 0.268 , 0.331	Depositor DCC
$R_{free}$ test set	1422 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	176.7	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 152.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.69	1/3345 (0.0%)	0.91	12/4513 (0.3%)
1	B	0.63	3/2980 (0.1%)	0.93	13/4018 (0.3%)
2	C	1.03	0/194	1.78	7/298 (2.3%)
All	All	0.68	4/6519 (0.1%)	0.96	32/8829 (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	B	1	1
2	C	1	1
All	All	2	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	CYS	CB-SG	18.27	2.13	1.82
1	B	1333	GLU	CB-CG	6.37	1.64	1.52
1	B	1333	GLU	CG-CD	5.35	1.59	1.51
1	B	1417	ALA	CA-CB	-5.20	1.41	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1395	PHE	CA-C-O	12.19	145.69	120.10
2	C	2009	DT	O4'-C4'-C3'	-10.88	99.47	106.00
2	C	2009	DT	O4'-C1'-N1	8.34	113.84	108.00
1	B	1379	ASP	CB-CG-OD1	7.96	125.46	118.30
2	C	2003	DT	O4'-C1'-N1	7.73	113.41	108.00
1	A	302	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	B	1176	LEU	CA-CB-CG	7.03	131.47	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	GLY	N-CA-C	7.02	130.65	113.10
1	B	1008	ARG	N-CA-C	-7.01	92.06	111.00
1	A	283	LEU	CA-CB-CG	-6.76	99.76	115.30
2	C	2008	DT	N1-C1'-C2'	6.68	125.30	112.60
1	A	324	LEU	CB-CG-CD1	-6.67	99.66	111.00
1	B	1009	ILE	N-CA-C	6.49	128.52	111.00
2	C	2008	DT	O4'-C1'-C2'	6.30	110.94	105.90
1	B	1333	GLU	N-CA-C	6.25	127.86	111.00
1	A	321	TYR	CA-CB-CG	6.08	124.95	113.40
1	B	1379	ASP	CB-CA-C	6.07	122.55	110.40
1	A	92	LEU	CA-CB-CG	-5.94	101.64	115.30
1	B	1395	PHE	N-CA-C	5.94	127.03	111.00
2	C	2008	DT	O4'-C1'-N1	5.73	112.01	108.00
1	A	408	ASN	N-CA-C	5.70	126.39	111.00
1	B	1083	VAL	CB-CA-C	-5.48	100.98	111.40
1	A	95	SER	N-CA-C	5.42	125.63	111.00
1	A	302	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	117	ARG	NE-CZ-NH1	-5.35	117.62	120.30
2	C	2005	DT	O4'-C1'-N1	5.30	111.71	108.00
1	B	1152	GLN	N-CA-C	5.29	125.29	111.00
1	B	1045	ARG	N-CA-C	5.26	125.21	111.00
1	A	333	GLU	N-CA-C	5.17	124.95	111.00
1	B	1214	VAL	N-CA-C	-5.12	97.19	111.00
1	A	407	GLU	N-CA-C	-5.08	97.28	111.00
1	B	1151	SER	N-CA-C	5.05	124.62	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	1415	ILE	CA
2	C	2008	DT	C1'

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1321	TYR	Sidechain
2	C	2009	DT	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	3310	0	3333	396	0
1	B	2952	0	2975	351	0
2	C	177	0	110	21	0
All	All	6439	0	6418	745	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 58.

All (745) 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:253:CYS:SG	1:A:253:CYS:CB	2.13	1.36
1:A:253:CYS:SG	1:A:260:ALA:HB2	1.75	1.24
1:B:1340:SER:CB	1:B:1388:GLN:HG2	1.68	1.22
1:A:335:ARG:HH21	1:A:338:GLU:HG2	1.10	1.12
1:B:1340:SER:HB2	1:B:1388:GLN:HG2	1.28	1.09
1:A:365:ARG:HB3	1:A:365:ARG:HH11	1.09	1.09
1:B:1333:GLU:OE1	1:B:1337:GLN:HG2	1.52	1.09
1:B:1380:LEU:CD1	1:B:1417:ALA:HB1	1.84	1.08
1:A:363:LEU:HD23	1:A:367:VAL:HG13	1.37	1.07
1:B:1340:SER:HB2	1:B:1388:GLN:CG	1.83	1.07
1:B:1051:ILE:HG12	1:B:1074:LEU:HD21	1.34	1.05
1:B:1219:PHE:HA	1:B:1222:ASN:HD22	1.20	1.05
1:A:365:ARG:HB3	1:A:365:ARG:NH1	1.72	1.05
1:A:77:LEU:HB3	1:A:79:GLN:HG3	1.37	1.04
1:A:398:ARG:HB3	1:A:412:ILE:HG12	1.38	1.04
1:A:192:GLU:HB3	1:A:427:VAL:HG13	1.39	1.03
1:A:321:TYR:CE2	1:A:324:LEU:HD11	1.94	1.02
1:B:1234:ASN:HB2	1:B:1314:LEU:HB2	1.42	1.02
1:A:253:CYS:SG	1:A:260:ALA:CB	2.50	1.00
1:A:268:LEU:HB2	1:A:273:TRP:CZ3	2.01	0.96
1:B:1391:ASP:HB3	1:B:1420:ARG:HG3	1.45	0.96
1:A:234:ASN:HB2	1:A:313:GLY:O	1.64	0.95
1:A:314:LEU:HD13	1:A:353:LEU:HD23	1.48	0.95
1:B:1333:GLU:CB	1:B:1337:GLN:HB3	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1101:ASN:HD22	1:B:1101:ASN:H	1.11	0.95
1:B:1384:GLY:O	1:B:1387:GLU:HG3	1.65	0.95
1:B:1380:LEU:HD11	1:B:1417:ALA:HB1	1.47	0.95
1:B:1188:THR:HG23	1:B:1190:PHE:H	1.31	0.95
1:A:315:GLY:O	1:A:355:VAL:HG13	1.68	0.94
1:A:321:TYR:CZ	1:A:324:LEU:HD11	2.03	0.92
1:B:1191:THR:HA	1:B:1194:ASP:HB2	1.51	0.92
1:B:1043:PHE:HD2	1:B:1048:HIS:HB3	1.35	0.91
1:A:326:GLN:NE2	2:C:2009:DT:H71	1.86	0.91
1:A:343:SER:HA	1:A:346:LEU:HD12	1.52	0.91
1:A:302:ARG:HH12	1:A:352:GLU:CD	1.75	0.90
1:A:216:LYS:HG2	1:A:217:THR:N	1.87	0.90
1:A:437:LYS:HG2	1:A:438:PHE:H	1.35	0.90
1:B:1024:VAL:HA	1:B:1030:ALA:HB3	1.51	0.89
1:A:321:TYR:CE1	1:A:324:LEU:HD21	2.08	0.89
2:C:2002:DT:H4'	2:C:2003:DT:OP2	1.73	0.88
1:A:239:SER:HA	1:A:320:ASP:HB3	1.54	0.87
1:A:257:ASN:OD1	1:A:437:LYS:NZ	2.07	0.87
1:A:321:TYR:HB3	1:A:362:GLN:NE2	1.88	0.87
1:B:1075:ALA:HB2	1:B:1080:LEU:HD22	1.56	0.87
1:B:1188:THR:HG21	1:B:1193:LEU:HB2	1.57	0.86
1:A:326:GLN:NE2	2:C:2009:DT:C7	2.37	0.86
1:A:216:LYS:HD2	1:A:362:GLN:HB3	1.58	0.85
1:A:363:LEU:HD21	1:A:366:SER:OG	1.74	0.85
1:B:1333:GLU:CD	1:B:1337:GLN:HG2	1.96	0.85
1:B:1391:ASP:O	1:B:1392:ILE:HG13	1.75	0.85
1:A:358:ILE:HG13	1:A:358:ILE:O	1.73	0.85
1:A:403:ASN:ND2	1:A:405:ASP:OD2	2.10	0.84
1:B:1340:SER:HB3	1:B:1388:GLN:HE21	1.43	0.84
1:A:212:PRO:HD3	1:A:367:VAL:CG2	2.09	0.83
1:A:335:ARG:NH2	1:A:338:GLU:HG2	1.92	0.83
1:B:1380:LEU:CD1	1:B:1417:ALA:CB	2.56	0.82
1:B:1415:ILE:HG23	1:B:1426:THR:OG1	1.79	0.82
1:A:227:VAL:O	1:A:231:THR:HG23	1.78	0.82
1:B:1031:LEU:HD13	1:B:1055:MET:HG2	1.62	0.82
1:A:219:PHE:CE1	1:A:223:ILE:HD11	2.15	0.82
1:B:1079:GLN:NE2	2:C:2004:DT:OP2	2.12	0.81
1:B:1340:SER:CB	1:B:1388:GLN:CG	2.48	0.81
1:A:413:GLU:HG2	1:A:428:GLN:HE21	1.45	0.81
1:B:1272:ASP:O	1:B:1276:LEU:HB2	1.80	0.81
1:B:1335:ARG:HH12	1:B:1383:SER:HA	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:VAL:HG13	1:A:63:GLU:HB3	1.61	0.80
1:A:212:PRO:HD3	1:A:367:VAL:HG21	1.62	0.80
1:A:225:GLN:OE1	1:A:255:GLU:HG2	1.82	0.80
1:B:1335:ARG:NH2	1:B:1384:GLY:H	1.80	0.80
1:A:136:ILE:HD12	1:A:137:ASP:N	1.97	0.80
1:A:314:LEU:HD23	1:A:315:GLY:N	1.97	0.80
1:B:1340:SER:HB3	1:B:1388:GLN:HG2	1.64	0.79
1:A:27:ASP:OD1	1:A:29:THR:HG23	1.83	0.79
1:A:320:ASP:HA	1:A:360:LEU:HD13	1.64	0.79
1:B:1105:TYR:O	1:B:1109:VAL:HG23	1.80	0.79
1:B:1330:ARG:NH2	2:C:2008:DT:H3	1.81	0.79
1:A:216:LYS:HE3	1:A:362:GLN:CD	2.03	0.79
1:A:203:SER:HA	1:A:350:ALA:O	1.83	0.78
1:A:21:LEU:HB2	1:A:92:LEU:HD22	1.63	0.78
1:B:1024:VAL:HG13	1:B:1031:LEU:HB2	1.65	0.78
1:B:1219:PHE:O	1:B:1222:ASN:HB2	1.82	0.78
1:B:1244:ALA:O	1:B:1248:VAL:HG12	1.83	0.78
1:A:102:VAL:HA	1:A:105:TYR:HD1	1.48	0.78
1:A:268:LEU:HB2	1:A:273:TRP:HZ3	1.49	0.78
1:B:1219:PHE:CA	1:B:1222:ASN:HD22	1.96	0.78
1:A:302:ARG:NH1	1:A:352:GLU:OE2	2.14	0.78
1:B:1384:GLY:HA2	1:B:1387:GLU:CG	2.14	0.77
1:A:211:ARG:HG2	1:A:367:VAL:HB	1.66	0.77
1:A:322:LEU:HD23	1:A:323:GLN:N	2.00	0.77
1:B:1101:ASN:ND2	1:B:1101:ASN:H	1.82	0.77
1:B:1333:GLU:HB3	1:B:1337:GLN:HB3	1.65	0.76
1:A:254:ALA:O	1:A:437:LYS:HE2	1.85	0.76
1:A:293:THR:HG23	1:A:294:PRO:HD2	1.66	0.76
1:A:33:LEU:O	1:A:36:GLU:HB2	1.85	0.76
2:C:2004:DT:H2'	2:C:2004:DT:O2	1.85	0.76
1:A:326:GLN:HE22	2:C:2009:DT:C7	1.99	0.76
1:B:1321:TYR:HA	1:B:1360:LEU:O	1.86	0.76
1:A:259:ASN:HB3	1:A:262:ASN:HB2	1.67	0.76
1:A:74:LEU:HD21	1:A:83:VAL:HG21	1.68	0.76
1:A:321:TYR:CD2	1:A:362:GLN:NE2	2.55	0.75
1:A:318:VAL:HB	1:A:358:ILE:HD11	1.66	0.75
1:B:1234:ASN:HB2	1:B:1314:LEU:CB	2.16	0.74
1:A:216:LYS:HG2	1:A:217:THR:H	1.50	0.74
1:A:377:MET:O	1:A:380:LEU:HD13	1.85	0.74
1:A:412:ILE:HD13	1:A:413:GLU:H	1.52	0.74
1:B:1221:LEU:HB3	1:B:1225:GLN:HE21	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1392:ILE:HA	1:B:1418:LYS:O	1.88	0.74
1:A:259:ASN:O	1:A:262:ASN:N	2.21	0.73
1:B:1384:GLY:C	1:B:1387:GLU:HG3	2.08	0.73
1:B:1211:ARG:HH21	1:B:1367:VAL:HB	1.53	0.73
1:A:79:GLN:O	1:A:82:GLU:HB3	1.89	0.73
1:A:315:GLY:O	1:A:355:VAL:CG1	2.37	0.73
1:B:1391:ASP:CB	1:B:1420:ARG:HG3	2.18	0.73
1:A:173:ILE:O	1:A:176:LEU:HB3	1.89	0.73
1:A:335:ARG:O	1:A:339:VAL:HG12	1.88	0.73
1:B:1380:LEU:HD12	1:B:1417:ALA:CB	2.18	0.72
1:A:412:ILE:HD13	1:A:413:GLU:N	2.04	0.72
1:B:1393:VAL:HG22	1:B:1417:ALA:HB3	1.71	0.72
1:B:1384:GLY:HA2	1:B:1387:GLU:HG3	1.70	0.72
1:A:40:PRO:HB2	1:A:41:GLU:OE1	1.89	0.72
1:A:331:ASN:CG	1:A:332:ARG:H	1.92	0.72
1:B:1222:ASN:O	1:B:1225:GLN:HB2	1.90	0.72
1:A:321:TYR:HB3	1:A:362:GLN:CD	2.10	0.72
1:A:102:VAL:HA	1:A:105:TYR:CD1	2.24	0.72
1:B:1043:PHE:CD2	1:B:1048:HIS:HB3	2.23	0.72
1:A:223:ILE:O	1:A:227:VAL:HG23	1.90	0.71
1:A:237:ILE:HA	1:A:318:VAL:HG13	1.72	0.71
1:A:113:SER:HA	1:A:116:ARG:NH2	2.04	0.71
1:A:118:LEU:CD1	1:A:150:VAL:HG11	2.19	0.71
1:B:1223:ILE:O	1:B:1227:VAL:HG23	1.90	0.71
1:B:1101:ASN:HD22	1:B:1102:VAL:H	1.38	0.71
1:A:239:SER:OG	1:A:242:MET:HB3	1.90	0.71
1:B:1333:GLU:HB2	1:B:1337:GLN:HB3	1.71	0.71
1:A:321:TYR:CB	1:A:362:GLN:HG3	2.20	0.71
1:A:58:VAL:CG1	1:A:63:GLU:HB3	2.21	0.70
1:B:1070:VAL:HG12	1:B:1071:THR:N	2.06	0.70
1:B:1365:ARG:H	1:B:1365:ARG:HD2	1.56	0.70
1:B:1092:LEU:O	1:B:1095:SER:HB3	1.91	0.70
1:A:406:SER:HA	1:A:408:ASN:ND2	2.07	0.70
1:A:69:THR:O	1:A:72:ALA:HB3	1.92	0.70
1:B:1322:LEU:HA	1:B:1325:ILE:HG13	1.73	0.70
1:A:412:ILE:HG22	1:A:429:LEU:O	1.92	0.69
1:A:227:VAL:HG13	1:A:231:THR:HG21	1.73	0.69
1:A:302:ARG:NH1	1:A:352:GLU:CD	2.46	0.69
1:A:31:LEU:HD21	1:A:56:LEU:HD12	1.73	0.69
1:A:247:LEU:HD22	1:A:290:ILE:HD13	1.75	0.69
1:B:1134:ASP:O	1:B:1135:GLU:HG3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1368:GLU:O	1:B:1372:ASP:OD2	2.11	0.69
1:A:40:PRO:HG3	1:A:52:PHE:HD2	1.56	0.69
1:A:118:LEU:HD13	1:A:150:VAL:HG11	1.75	0.68
1:B:1298:VAL:HA	1:B:1301:ILE:HD12	1.75	0.68
1:B:1340:SER:HB3	1:B:1388:GLN:NE2	2.07	0.68
1:B:1211:ARG:HH21	1:B:1367:VAL:CB	2.06	0.68
1:B:1271:GLU:O	1:B:1275:LYS:HG2	1.94	0.68
1:B:1325:ILE:HB	1:B:1342:ILE:HD13	1.76	0.68
1:A:258:ILE:HD11	1:A:276:LEU:HA	1.75	0.68
1:A:326:GLN:HE22	2:C:2009:DT:H71	1.59	0.68
1:A:216:LYS:HD2	1:A:362:GLN:CB	2.22	0.68
1:B:1238:PHE:CE2	1:B:1301:ILE:HG23	2.28	0.68
1:A:321:TYR:HD1	1:A:323:GLN:HG2	1.59	0.67
1:B:1051:ILE:HG12	1:B:1074:LEU:CD2	2.20	0.67
1:B:1380:LEU:HD11	1:B:1417:ALA:CB	2.24	0.67
1:A:269:THR:HB	1:A:270:PRO:HD2	1.74	0.67
1:B:1024:VAL:HG21	1:B:1055:MET:CE	2.24	0.67
1:B:1220:ALA:HB2	1:B:1360:LEU:HD11	1.75	0.67
1:A:220:ALA:HB2	1:A:360:LEU:HD21	1.75	0.67
1:B:1363:LEU:HD11	1:B:1395:PHE:HE1	1.60	0.67
1:A:355:VAL:HG13	1:A:356:PRO:HD2	1.75	0.67
1:B:1335:ARG:NH1	1:B:1383:SER:HA	2.10	0.67
1:B:1290:ILE:HG22	1:B:1291:ASP:H	1.60	0.67
1:B:1319:ILE:O	1:B:1360:LEU:HG	1.93	0.67
1:A:238:PHE:CD2	1:A:319:ILE:HG12	2.30	0.67
1:B:1224:ALA:HB2	1:B:1318:VAL:HG21	1.76	0.67
1:B:1188:THR:HG23	1:B:1190:PHE:N	2.09	0.66
1:B:1249:MET:O	1:B:1253:CYS:HB2	1.95	0.66
1:B:1393:VAL:CG2	1:B:1417:ALA:HB3	2.26	0.66
1:B:1340:SER:CA	1:B:1388:GLN:HG2	2.25	0.66
1:B:1384:GLY:CA	1:B:1387:GLU:HG3	2.26	0.66
1:B:1125:ILE:O	1:B:1128:ASP:HB2	1.96	0.66
1:A:238:PHE:HD2	1:A:319:ILE:HG12	1.61	0.66
1:B:1333:GLU:OE1	1:B:1337:GLN:CG	2.39	0.66
1:B:1101:ASN:O	1:B:1104:TYR:N	2.20	0.66
1:A:21:LEU:HD22	1:A:55:MET:CE	2.26	0.65
1:B:1188:THR:HG22	1:B:1194:ASP:CG	2.15	0.65
1:B:1208:VAL:HG23	1:B:1208:VAL:O	1.96	0.65
1:A:206:ILE:HB	1:A:358:ILE:HA	1.78	0.65
1:B:1090:SER:O	1:B:1093:ALA:HB3	1.96	0.65
1:A:428:GLN:O	1:A:429:LEU:HD12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:HH22	1:A:107:ARG:HE	1.43	0.65
1:A:188:THR:HB	1:A:194:ASP:OD2	1.97	0.65
1:A:188:THR:O	1:A:190:PHE:N	2.30	0.65
1:B:1290:ILE:HG22	1:B:1291:ASP:N	2.11	0.65
1:B:1080:LEU:O	1:B:1083:VAL:HG22	1.97	0.64
1:B:1166:LEU:O	1:B:1169:THR:N	2.30	0.64
1:A:238:PHE:CB	1:A:319:ILE:HG23	2.27	0.64
1:A:321:TYR:HB3	1:A:362:GLN:CG	2.28	0.64
1:A:12:GLN:OE1	1:A:44:TYR:CE2	2.50	0.64
1:A:208:VAL:O	1:A:360:LEU:HA	1.98	0.64
1:B:1107:ARG:O	1:B:1111:GLU:HG2	1.98	0.64
1:A:321:TYR:HB2	1:A:362:GLN:HG3	1.78	0.64
1:B:1272:ASP:HA	1:B:1275:LYS:HG2	1.80	0.64
1:B:1211:ARG:NH2	1:B:1367:VAL:HB	2.13	0.64
1:A:170:TYR:HA	1:A:173:ILE:HG22	1.80	0.64
1:B:1187:PRO:HA	1:B:1194:ASP:OD1	1.98	0.64
1:B:1221:LEU:HD11	1:B:1247:LEU:HD11	1.80	0.63
1:B:1031:LEU:CD1	1:B:1055:MET:HG2	2.29	0.63
1:B:1037:ARG:HH21	1:B:1107:ARG:HH12	1.44	0.63
1:B:1217:THR:O	1:B:1221:LEU:HD22	1.98	0.63
1:A:202:ARG:O	1:A:203:SER:HB2	1.99	0.63
1:A:193:LEU:HA	1:A:427:VAL:HG21	1.81	0.63
1:B:1252:LEU:HA	1:B:1255:GLU:HB3	1.79	0.63
1:B:1340:SER:HB2	1:B:1388:GLN:HG3	1.78	0.63
1:A:283:LEU:HA	1:A:286:ALA:HB2	1.81	0.63
1:A:21:LEU:CB	1:A:92:LEU:HD22	2.29	0.62
1:A:13:SER:O	1:A:17:GLU:HG3	1.99	0.62
1:B:1031:LEU:HD22	1:B:1065:VAL:HG11	1.78	0.62
1:A:299:SER:HB3	1:B:1036:GLU:O	1.99	0.62
1:A:326:GLN:HE21	2:C:2009:DT:H71	1.65	0.62
1:A:283:LEU:O	1:A:286:ALA:N	2.31	0.62
1:B:1024:VAL:HG21	1:B:1055:MET:HE3	1.81	0.62
1:B:1134:ASP:C	1:B:1135:GLU:HG3	2.20	0.62
1:B:1326:GLN:HE21	1:B:1331:ASN:HD21	1.47	0.62
1:B:1328:SER:HB3	1:B:1338:GLU:OE1	1.99	0.62
1:A:242:MET:HG3	1:A:246:GLN:HE21	1.63	0.62
1:B:1039:ILE:O	1:B:1040:PRO:C	2.37	0.62
1:A:238:PHE:HB2	1:A:319:ILE:HG23	1.82	0.62
1:B:1110:GLU:O	1:B:1113:SER:HB3	2.00	0.62
1:A:437:LYS:HG2	1:A:438:PHE:N	2.11	0.61
1:A:154:LYS:O	1:A:156:SER:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLN:NE2	2:C:2009:DT:H72	2.16	0.61
1:A:146:LYS:O	1:A:149:GLU:HB2	2.01	0.61
1:A:21:LEU:HD22	1:A:55:MET:HE1	1.82	0.61
1:A:283:LEU:HA	1:A:286:ALA:CB	2.31	0.61
1:A:298:VAL:HB	1:A:342:ILE:HG12	1.83	0.61
1:A:212:PRO:HB2	1:A:368:GLU:OE1	2.00	0.61
1:B:1101:ASN:HD22	1:B:1102:VAL:N	1.97	0.61
1:A:112:LYS:O	1:A:116:ARG:HG3	2.01	0.61
1:A:71:THR:HG23	1:A:86:VAL:HG12	1.82	0.61
1:B:1391:ASP:CG	1:B:1420:ARG:HD2	2.21	0.61
1:A:224:ALA:HB1	1:A:235:VAL:HG11	1.83	0.60
1:A:335:ARG:HA	1:A:338:GLU:HB3	1.82	0.60
1:B:1053:HIS:O	1:B:1054:ALA:C	2.39	0.60
1:A:318:VAL:HG13	1:A:318:VAL:O	2.01	0.60
1:A:18:GLN:NE2	1:A:95:SER:OG	2.34	0.60
1:B:1070:VAL:HG13	1:B:1074:LEU:HD13	1.83	0.60
1:B:1347:LYS:HZ1	1:B:1420:ARG:HH12	1.48	0.60
1:B:1024:VAL:CG1	1:B:1031:LEU:HB2	2.31	0.60
1:B:1170:TYR:O	1:B:1173:ILE:HG22	2.01	0.60
1:B:1325:ILE:O	1:B:1325:ILE:HG22	2.02	0.60
1:A:206:ILE:HD12	1:A:356:PRO:HB2	1.84	0.60
1:B:1045:ARG:NH1	2:C:2006:DT:H73	2.17	0.60
1:A:263:LEU:HA	1:A:268:LEU:HD21	1.83	0.60
1:B:1296:ILE:HG12	1:B:1297:ARG:N	2.17	0.59
1:A:219:PHE:O	1:A:223:ILE:HG13	2.02	0.59
1:B:1101:ASN:HD22	1:B:1101:ASN:N	1.83	0.59
1:B:1195:ARG:HD2	1:B:1196:MET:HG2	1.84	0.59
1:B:1251:MET:HB3	1:B:1283:LEU:HD21	1.84	0.59
1:A:249:MET:O	1:A:253:CYS:SG	2.58	0.59
1:B:1386:ILE:HD12	1:B:1393:VAL:HG11	1.83	0.59
1:A:238:PHE:HB2	1:A:319:ILE:HA	1.85	0.59
1:A:326:GLN:HE22	2:C:2009:DT:H72	1.68	0.59
1:A:216:LYS:HD2	1:A:362:GLN:CG	2.33	0.59
1:A:57:ARG:HH22	1:A:77:LEU:HD23	1.68	0.59
1:B:1048:HIS:O	1:B:1049:GLN:C	2.39	0.59
1:B:1347:LYS:NZ	1:B:1420:ARG:HH12	1.99	0.59
1:A:121:THR:O	1:A:125:ILE:HG13	2.02	0.59
1:A:220:ALA:HB1	1:A:318:VAL:HG21	1.85	0.59
1:A:331:ASN:ND2	1:A:332:ARG:H	2.01	0.59
1:A:420:ARG:NH1	1:A:421:ASN:OD1	2.36	0.59
1:A:104:TYR:O	1:A:108:ILE:HG13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:THR:CG2	1:A:296:ILE:HG12	2.34	0.58
1:B:1211:ARG:HB3	1:B:1367:VAL:HG21	1.83	0.58
1:A:13:SER:HB3	1:A:16:ALA:HB3	1.85	0.58
1:A:274:GLY:O	1:A:278:MET:N	2.36	0.58
1:A:216:LYS:CE	1:A:362:GLN:CD	2.72	0.58
1:A:258:ILE:O	1:A:435:TYR:HD1	1.86	0.58
1:A:249:MET:SD	1:A:263:LEU:HD23	2.44	0.58
1:A:368:GLU:O	1:A:371:GLN:NE2	2.36	0.58
1:B:1220:ALA:CB	1:B:1360:LEU:HD11	2.33	0.58
1:A:418:LYS:HG2	1:A:419:GLN:N	2.18	0.58
1:B:1169:THR:HG22	1:B:1169:THR:O	2.03	0.58
1:B:1341:GLU:O	1:B:1345:SER:HB2	2.04	0.58
1:B:1137:ASP:HB3	1:B:1297:ARG:HH22	1.67	0.58
1:A:167:VAL:HG23	1:A:168:GLN:N	2.18	0.58
1:A:193:LEU:O	1:A:196:MET:N	2.35	0.58
1:A:367:VAL:HG23	1:A:368:GLU:N	2.18	0.58
1:A:411:ILE:HG23	1:A:411:ILE:O	2.04	0.58
1:B:1024:VAL:CA	1:B:1030:ALA:HB3	2.29	0.58
1:B:1211:ARG:HE	1:B:1367:VAL:HG21	1.69	0.58
1:A:220:ALA:CB	1:A:360:LEU:HD21	2.33	0.58
1:B:1322:LEU:HB2	1:B:1325:ILE:HD12	1.86	0.58
1:B:1343:SER:O	1:B:1346:LEU:HB2	2.03	0.58
1:A:274:GLY:O	1:A:275:LYS:C	2.39	0.57
1:A:318:VAL:HA	1:A:358:ILE:HG13	1.86	0.57
1:B:1321:TYR:CE1	1:B:1324:LEU:HG	2.39	0.57
1:A:269:THR:H	1:A:272:ASP:HB2	1.69	0.57
1:A:319:ILE:O	1:A:360:LEU:HD12	2.05	0.57
1:A:406:SER:HA	1:A:408:ASN:HD22	1.69	0.57
1:B:1302:ARG:HB3	1:B:1349:LEU:HD13	1.86	0.57
1:A:321:TYR:HB3	1:A:362:GLN:HG3	1.85	0.57
1:A:212:PRO:HG3	1:A:363:LEU:O	2.05	0.57
1:B:1224:ALA:HB1	1:B:1235:VAL:HG21	1.86	0.57
1:A:70:VAL:HG13	1:A:71:THR:N	2.19	0.57
1:A:207:ILE:CD1	1:A:386:ILE:HG22	2.33	0.57
1:A:274:GLY:HA2	1:A:277:THR:OG1	2.05	0.57
1:A:380:LEU:HD12	1:A:395:PHE:HZ	1.70	0.57
1:A:368:GLU:O	1:A:371:GLN:HG3	2.05	0.56
1:A:211:ARG:CG	1:A:367:VAL:HB	2.34	0.56
1:A:211:ARG:HB3	1:A:212:PRO:CD	2.35	0.56
1:B:1247:LEU:HD23	1:B:1290:ILE:HD13	1.86	0.56
1:A:106:ALA:O	1:A:109:VAL:HB	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:MET:SD	1:A:263:LEU:CD2	2.93	0.56
1:A:41:GLU:OE1	1:A:41:GLU:N	2.37	0.56
1:B:1384:GLY:HA2	1:B:1387:GLU:HG2	1.87	0.56
1:A:206:ILE:HA	1:A:392:ILE:HG23	1.88	0.56
1:A:323:GLN:NE2	1:A:361:SER:HA	2.21	0.56
1:B:1088:TYR:O	1:B:1091:GLU:HB2	2.06	0.56
1:A:380:LEU:HD21	1:A:387:GLU:HB2	1.87	0.56
1:A:427:VAL:HG12	1:A:428:GLN:N	2.20	0.56
1:A:67:LEU:O	1:A:70:VAL:HG12	2.05	0.56
1:B:1056:LEU:O	1:B:1059:ALA:HB3	2.06	0.56
1:B:1365:ARG:N	1:B:1365:ARG:HD2	2.20	0.56
1:A:289:TYR:CE2	1:A:308:LEU:HD11	2.41	0.56
1:A:360:LEU:N	1:A:360:LEU:HD12	2.20	0.56
1:A:377:MET:HE1	1:A:387:GLU:HG3	1.87	0.56
1:B:1302:ARG:HG3	1:B:1303:ALA:N	2.19	0.56
1:B:1326:GLN:HE21	1:B:1331:ASN:ND2	2.03	0.56
1:B:1240:LEU:HD21	1:B:1296:ILE:HG22	1.88	0.56
1:B:1299:SER:O	1:B:1302:ARG:HG3	2.06	0.56
1:B:1080:LEU:HA	1:B:1083:VAL:HG22	1.87	0.55
1:A:293:THR:CG2	1:A:294:PRO:HD2	2.34	0.55
1:A:321:TYR:CD2	1:A:362:GLN:CD	2.79	0.55
1:B:1073:GLU:O	1:B:1076:ALA:HB3	2.07	0.55
1:A:183:ILE:HG22	1:A:185:GLY:H	1.71	0.55
1:A:24:VAL:HA	1:A:30:ALA:HB3	1.87	0.55
1:A:236:ALA:O	1:A:318:VAL:HG12	2.06	0.55
1:A:207:ILE:O	1:A:393:VAL:HA	2.07	0.55
1:A:86:VAL:O	1:A:89:LEU:N	2.39	0.55
1:B:1157:GLY:HA2	1:B:1351:ARG:NH1	2.22	0.55
1:A:283:LEU:O	1:A:284:SER:C	2.43	0.55
1:A:321:TYR:CE1	1:A:324:LEU:CD2	2.88	0.55
1:A:360:LEU:HD12	1:A:360:LEU:H	1.72	0.55
1:B:1052:PHE:O	1:B:1055:MET:HB3	2.06	0.55
1:A:153:ARG:HG3	1:A:153:ARG:HH21	1.71	0.55
1:B:1247:LEU:CD2	1:B:1290:ILE:HD13	2.37	0.55
1:A:259:ASN:O	1:A:262:ASN:HB2	2.07	0.55
1:A:321:TYR:CZ	1:A:324:LEU:HD21	2.41	0.55
1:A:328:SER:O	1:A:329:GLY:O	2.25	0.55
1:B:1045:ARG:NH1	2:C:2006:DT:C7	2.70	0.55
1:A:212:PRO:HD3	1:A:367:VAL:HG23	1.88	0.54
1:B:1102:VAL:HG13	1:B:1103:GLU:N	2.22	0.54
1:B:1131:THR:O	1:B:1131:THR:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLY:O	1:A:275:LYS:HD3	2.07	0.54
1:B:1054:ALA:CB	1:B:1074:LEU:CD1	2.86	0.54
1:B:1206:ILE:N	1:B:1206:ILE:HD12	2.20	0.54
1:B:1219:PHE:HA	1:B:1222:ASN:ND2	2.06	0.54
1:B:1211:ARG:HE	1:B:1367:VAL:CG2	2.19	0.54
1:A:118:LEU:HD12	1:A:150:VAL:HG11	1.89	0.54
1:A:302:ARG:HD2	1:B:1036:GLU:OE1	2.07	0.54
1:A:66:ASP:OD2	1:A:69:THR:OG1	2.22	0.54
1:A:67:LEU:C	1:A:67:LEU:HD23	2.27	0.54
1:A:261:GLN:HA	1:A:264:ARG:HG2	1.89	0.54
1:A:206:ILE:O	1:A:359:ALA:N	2.37	0.54
1:A:220:ALA:HB1	1:A:318:VAL:CG2	2.38	0.54
1:A:318:VAL:CB	1:A:358:ILE:HD11	2.36	0.54
1:B:1235:VAL:HG12	1:B:1316:MET:HB3	1.89	0.54
1:A:223:ILE:O	1:A:224:ALA:C	2.45	0.54
1:B:1299:SER:HA	1:B:1302:ARG:HG2	1.89	0.54
1:B:1296:ILE:HG23	1:B:1325:ILE:HG23	1.90	0.54
1:A:413:GLU:HG2	1:A:428:GLN:NE2	2.21	0.54
1:A:25:PHE:CZ	1:A:89:LEU:HD22	2.43	0.54
1:A:330:ARG:NH2	1:B:1041:GLU:CD	2.61	0.54
1:A:242:MET:HG3	1:A:246:GLN:NE2	2.23	0.53
1:B:1040:PRO:HG2	1:B:1053:HIS:HD2	1.73	0.53
1:B:1211:ARG:HH21	1:B:1367:VAL:C	2.11	0.53
1:B:1296:ILE:CD1	1:B:1301:ILE:HG12	2.37	0.53
1:B:1338:GLU:O	1:B:1342:ILE:HG13	2.08	0.53
1:B:1350:ALA:HB2	1:B:1357:VAL:CG2	2.39	0.53
1:B:1132:ARG:HD2	1:B:1135:GLU:OE1	2.08	0.53
1:B:1165:VAL:O	1:B:1166:LEU:C	2.44	0.53
1:B:1344:ARG:HA	1:B:1389:ASP:OD2	2.09	0.53
1:A:216:LYS:HE3	1:A:362:GLN:NE2	2.22	0.53
1:A:216:LYS:NZ	1:A:362:GLN:OE1	2.39	0.53
1:B:1126:ALA:O	1:B:1128:ASP:N	2.42	0.53
1:A:21:LEU:HD13	1:A:51:ILE:HG21	1.90	0.53
1:A:51:ILE:O	1:A:55:MET:HG3	2.09	0.53
1:A:188:THR:O	1:A:188:THR:HG22	2.08	0.53
1:A:321:TYR:CG	1:A:362:GLN:CD	2.82	0.53
1:A:27:ASP:CG	1:A:29:THR:HG23	2.28	0.53
1:A:264:ARG:HG3	1:A:265:THR:N	2.24	0.52
1:A:380:LEU:HD22	1:A:380:LEU:C	2.29	0.52
1:B:1321:TYR:CD1	1:B:1323:GLN:HG2	2.44	0.52
1:A:321:TYR:HB3	1:A:362:GLN:HE21	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:VAL:HG21	1:B:1055:MET:HE1	1.92	0.52
1:B:1038:LEU:HA	1:B:1042:ASP:OD1	2.10	0.52
1:B:1346:LEU:O	1:B:1347:LYS:C	2.48	0.52
1:A:211:ARG:HB3	1:A:212:PRO:HD2	1.92	0.52
1:A:252:LEU:HD23	1:A:276:LEU:HD12	1.90	0.52
1:A:77:LEU:O	1:A:78:GLU:HB2	2.08	0.52
1:A:302:ARG:NH1	1:B:1033:LEU:HD21	2.25	0.52
1:B:1416:ILE:CD1	1:B:1419:GLN:NE2	2.73	0.52
1:B:1043:PHE:CZ	1:B:1052:PHE:HD2	2.27	0.52
1:B:1054:ALA:O	1:B:1055:MET:C	2.48	0.52
1:A:321:TYR:CB	1:A:362:GLN:CG	2.87	0.52
1:A:57:ARG:NH2	1:A:77:LEU:HD23	2.24	0.52
1:B:1183:ILE:O	1:B:1183:ILE:HG23	2.11	0.51
1:B:1321:TYR:HD1	1:B:1323:GLN:HG2	1.75	0.51
1:A:321:TYR:CB	1:A:362:GLN:CD	2.78	0.51
1:B:1023:ALA:O	1:B:1024:VAL:C	2.46	0.51
1:B:1211:ARG:HH22	1:B:1371:GLN:HB2	1.75	0.51
1:A:394:ALA:HA	1:A:416:ILE:HA	1.92	0.51
1:A:86:VAL:HA	1:A:89:LEU:HD12	1.92	0.51
1:A:411:ILE:HD11	1:A:428:GLN:CD	2.30	0.51
1:B:1271:GLU:HG2	1:B:1275:LYS:NZ	2.24	0.51
1:A:237:ILE:HB	1:A:290:ILE:HG23	1.93	0.51
1:A:80:LEU:C	1:A:82:GLU:N	2.61	0.51
1:B:1055:MET:HG3	1:B:1065:VAL:HG21	1.91	0.51
1:B:1066:ASP:OD1	1:B:1066:ASP:O	2.28	0.51
1:B:1220:ALA:HB2	1:B:1360:LEU:CD1	2.41	0.51
1:B:1025:PHE:HD1	1:B:1093:ALA:HB2	1.75	0.51
1:A:356:PRO:O	1:A:356:PRO:HG2	2.11	0.51
1:B:1101:ASN:N	1:B:1101:ASN:ND2	2.47	0.51
1:B:1198:SER:O	1:B:1198:SER:OG	2.27	0.51
1:B:1251:MET:HB3	1:B:1283:LEU:CD2	2.41	0.51
1:A:202:ARG:HD2	1:A:354:GLU:O	2.10	0.51
1:A:369:GLN:HA	1:A:371:GLN:NE2	2.25	0.51
1:B:1146:LYS:HZ1	2:C:2007:DT:H3	1.57	0.51
1:A:212:PRO:O	1:A:213:SER:HB2	2.11	0.50
1:B:1170:TYR:HA	1:B:1173:ILE:HG22	1.94	0.50
1:A:227:VAL:HG21	1:A:316:MET:HE2	1.94	0.50
1:A:259:ASN:O	1:A:260:ALA:C	2.50	0.50
1:A:31:LEU:HD21	1:A:56:LEU:CD1	2.40	0.50
1:B:1087:SER:O	1:B:1091:GLU:HG3	2.11	0.50
1:B:1217:THR:HG22	1:B:1221:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:HH12	1:A:107:ARG:CZ	2.24	0.50
1:A:206:ILE:O	1:A:358:ILE:HA	2.12	0.50
1:B:1322:LEU:CD2	1:B:1322:LEU:H	2.24	0.50
1:A:134:ASP:OD1	1:A:135:GLU:HG3	2.12	0.50
1:A:136:ILE:HD12	1:A:136:ILE:C	2.32	0.50
1:B:1234:ASN:OD1	1:B:1313:GLY:O	2.30	0.50
1:B:1325:ILE:O	1:B:1327:GLY:N	2.45	0.50
1:A:238:PHE:HB3	1:A:319:ILE:HG23	1.94	0.50
1:A:252:LEU:HG	1:A:279:ALA:HB3	1.93	0.50
1:A:237:ILE:HG12	1:A:318:VAL:CG1	2.41	0.50
1:A:428:GLN:C	1:A:429:LEU:HD12	2.32	0.50
1:B:1016:ALA:O	1:B:1019:ALA:HB3	2.12	0.50
1:A:337:GLN:O	1:A:340:SER:HB2	2.11	0.49
1:A:434:GLU:OE1	1:A:434:GLU:N	2.45	0.49
1:A:243:SER:H	1:A:246:GLN:NE2	2.11	0.49
1:A:302:ARG:NE	1:A:349:LEU:HD12	2.26	0.49
1:B:1101:ASN:ND2	1:B:1102:VAL:N	2.60	0.49
1:B:1231:THR:CG2	1:B:1233:GLU:HG2	2.42	0.49
1:B:1054:ALA:O	1:B:1055:MET:O	2.30	0.49
1:B:1054:ALA:HB3	1:B:1074:LEU:HD11	1.94	0.49
1:B:1363:LEU:HD11	1:B:1395:PHE:CE1	2.45	0.49
1:A:326:GLN:HE21	2:C:2009:DT:C7	2.21	0.49
1:A:319:ILE:O	1:A:360:LEU:CD1	2.60	0.49
1:A:315:GLY:O	1:A:356:PRO:HD2	2.13	0.49
1:B:1344:ARG:CZ	2:C:2009:DT:O2	2.60	0.49
1:B:1296:ILE:HD13	1:B:1301:ILE:HG12	1.94	0.49
1:A:293:THR:HB	1:A:296:ILE:HD11	1.94	0.49
1:B:1140:LEU:O	1:B:1144:GLU:HG3	2.13	0.49
1:A:37:ARG:NH2	1:A:107:ARG:HE	2.10	0.49
1:A:196:MET:SD	1:A:427:VAL:HG23	2.53	0.49
1:B:1079:GLN:O	1:B:1083:VAL:HG13	2.13	0.49
1:B:1118:LEU:C	1:B:1118:LEU:HD13	2.33	0.49
1:B:1217:THR:HG22	1:B:1221:LEU:HD22	1.95	0.49
1:B:1346:LEU:O	1:B:1349:LEU:HB3	2.13	0.49
1:A:205:LEU:HD21	1:A:346:LEU:HB3	1.94	0.49
1:A:380:LEU:O	1:A:383:SER:HB2	2.12	0.49
1:B:1280:MET:HG3	1:B:1281:GLY:N	2.28	0.49
1:A:113:SER:O	1:A:116:ARG:HB2	2.13	0.49
1:B:1206:ILE:HB	1:B:1358:ILE:HA	1.94	0.49
1:B:1054:ALA:CB	1:B:1074:LEU:HD12	2.43	0.48
1:A:239:SER:HA	1:A:320:ASP:CB	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:MET:O	1:A:281:GLY:C	2.50	0.48
1:A:283:LEU:HG	1:A:283:LEU:H	1.23	0.48
1:A:180:ASN:OD1	1:A:195:ARG:NH2	2.46	0.48
1:B:1238:PHE:CZ	1:B:1301:ILE:HG23	2.49	0.48
1:B:1336:GLN:O	1:B:1340:SER:HB3	2.13	0.48
1:B:1107:ARG:HH21	1:B:1107:ARG:HG3	1.78	0.48
1:B:1333:GLU:HB3	1:B:1337:GLN:CB	2.42	0.48
1:A:55:MET:O	1:A:56:LEU:C	2.51	0.48
1:A:303:ALA:O	1:A:307:ARG:HG3	2.14	0.48
1:B:1347:LYS:NZ	1:B:1420:ARG:NH1	2.62	0.48
2:C:2004:DT:O2	2:C:2004:DT:C2'	2.58	0.48
1:B:1075:ALA:HA	1:B:1080:LEU:HB2	1.96	0.47
1:B:1300:ASP:O	1:B:1303:ALA:HB3	2.15	0.47
1:A:209:ALA:HA	1:A:361:SER:O	2.15	0.47
1:A:318:VAL:HA	1:A:358:ILE:CG1	2.44	0.47
1:B:1033:LEU:HD22	1:B:1036:GLU:OE2	2.14	0.47
1:B:1322:LEU:H	1:B:1322:LEU:HD23	1.79	0.47
1:A:377:MET:CE	1:A:387:GLU:HG3	2.44	0.47
1:A:99:ALA:O	1:A:102:VAL:N	2.35	0.47
1:A:268:LEU:HB2	1:A:273:TRP:CE3	2.46	0.47
1:A:21:LEU:HB2	1:A:92:LEU:CD2	2.41	0.47
1:A:248:VAL:HG21	1:B:1165:VAL:HG21	1.95	0.47
1:A:89:LEU:HA	1:A:92:LEU:HB2	1.96	0.47
1:B:1426:THR:HG22	1:B:1427:VAL:N	2.29	0.47
1:B:1066:ASP:C	1:B:1066:ASP:OD1	2.52	0.47
1:A:339:VAL:HG13	1:A:340:SER:N	2.30	0.47
1:B:1128:ASP:O	1:B:1129:GLY:C	2.52	0.47
1:B:1296:ILE:CG1	1:B:1297:ARG:N	2.77	0.47
1:B:1390:ALA:O	1:B:1418:LYS:HD3	2.15	0.47
1:B:1330:ARG:CZ	2:C:2008:DT:H3	2.27	0.47
1:B:1188:THR:HG21	1:B:1193:LEU:CB	2.36	0.47
1:A:107:ARG:O	1:A:110:GLU:N	2.48	0.47
1:A:17:GLU:OE1	1:A:43:PHE:HA	2.14	0.47
1:A:207:ILE:HD12	1:A:386:ILE:HG22	1.96	0.47
1:A:439:VAL:HG12	1:A:440:ASN:O	2.15	0.47
1:A:14:ILE:O	1:A:17:GLU:N	2.48	0.47
1:B:1045:ARG:HD2	1:B:1046:ALA:H	1.80	0.47
1:B:1269:THR:O	1:B:1272:ASP:HB2	2.14	0.47
1:B:1235:VAL:HG12	1:B:1316:MET:CB	2.44	0.47
1:B:1055:MET:O	1:B:1056:LEU:C	2.53	0.47
1:B:1211:ARG:NH2	1:B:1367:VAL:C	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1415:ILE:CG2	1:B:1426:THR:OG1	2.57	0.46
1:A:367:VAL:HG23	1:A:368:GLU:H	1.80	0.46
1:A:80:LEU:C	1:A:82:GLU:H	2.18	0.46
1:B:1178:ASN:O	1:B:1179:ARG:HB3	2.15	0.46
1:A:153:ARG:HG3	1:A:153:ARG:NH2	2.30	0.46
1:A:251:MET:SD	1:A:288:ILE:HD13	2.56	0.46
1:A:363:LEU:HG	1:A:364:SER:H	1.80	0.46
1:B:1188:THR:HG21	1:B:1194:ASP:N	2.31	0.46
1:B:1365:ARG:O	1:B:1369:GLN:HB2	2.16	0.46
1:A:167:VAL:HG23	1:A:168:GLN:H	1.81	0.46
1:A:335:ARG:HH21	1:A:338:GLU:CG	2.03	0.46
1:A:216:LYS:CE	1:A:362:GLN:OE1	2.63	0.46
1:A:46:ALA:O	1:A:49:GLN:HB2	2.15	0.46
1:A:54:ALA:O	1:A:57:ARG:HB2	2.16	0.46
1:A:16:ALA:O	1:A:17:GLU:C	2.52	0.46
1:A:179:ARG:HA	1:A:179:ARG:HD2	1.64	0.46
1:A:253:CYS:SG	1:A:260:ALA:HB1	2.50	0.46
1:A:260:ALA:O	1:A:263:LEU:N	2.49	0.46
1:A:98:THR:HG23	1:A:98:THR:O	2.16	0.46
1:B:1178:ASN:HD22	1:B:1178:ASN:HA	1.57	0.46
1:B:1037:ARG:HE	1:B:1107:ARG:NH1	2.13	0.46
1:A:322:LEU:CD2	1:A:323:GLN:NE2	2.79	0.46
1:A:219:PHE:CE2	1:A:414:ILE:HD11	2.51	0.46
1:A:273:TRP:O	1:A:277:THR:OG1	2.28	0.46
1:B:1251:MET:SD	1:B:1288:ILE:HD12	2.56	0.46
1:A:237:ILE:HG23	1:A:318:VAL:HG13	1.97	0.46
1:A:412:ILE:HG21	1:A:438:PHE:HE2	1.79	0.46
1:A:72:ALA:O	1:A:73:GLU:C	2.55	0.45
1:A:74:LEU:HD23	1:A:80:LEU:HD23	1.97	0.45
1:A:25:PHE:HZ	1:A:89:LEU:HD22	1.79	0.45
1:B:1393:VAL:HG13	1:B:1418:LYS:HB3	1.98	0.45
1:A:212:PRO:HG3	1:A:364:SER:HA	1.99	0.45
1:A:70:VAL:O	1:A:74:LEU:HB2	2.16	0.45
1:B:1054:ALA:HB1	1:B:1074:LEU:HD12	1.99	0.45
1:B:1061:LYS:NZ	1:B:1073:GLU:OE1	2.48	0.45
1:B:1208:VAL:O	1:B:1208:VAL:CG2	2.64	0.45
1:B:1322:LEU:CA	1:B:1325:ILE:HG13	2.44	0.45
1:A:107:ARG:O	1:A:110:GLU:HB3	2.16	0.45
1:A:216:LYS:HE3	1:A:362:GLN:OE1	2.16	0.45
1:B:1088:TYR:CZ	1:B:1092:LEU:HD21	2.51	0.45
1:B:1121:THR:HG22	1:B:1122:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1226:ASN:OD1	1:B:1226:ASN:N	2.47	0.45
1:B:1353:LEU:HB3	1:B:1355:VAL:HG22	1.98	0.45
1:A:301:ILE:O	1:A:305:CYS:SG	2.70	0.45
1:A:80:LEU:O	1:A:82:GLU:N	2.49	0.45
1:B:1186:ILE:O	1:B:1186:ILE:HG22	2.16	0.45
1:B:1249:MET:SD	1:B:1253:CYS:SG	3.00	0.45
1:A:262:ASN:HA	1:A:262:ASN:HD22	1.58	0.45
1:A:273:TRP:CZ2	1:B:1177:HIS:ND1	2.85	0.45
1:A:325:ILE:HG21	1:A:342:ILE:HD13	1.98	0.45
1:B:1252:LEU:HD12	1:B:1252:LEU:C	2.37	0.45
1:B:1137:ASP:CB	1:B:1297:ARG:HH22	2.30	0.45
1:B:1008:ARG:HD3	1:B:1008:ARG:HA	1.76	0.45
1:B:1088:TYR:CE1	1:B:1092:LEU:HD11	2.51	0.45
1:B:1104:TYR:CD1	1:B:1105:TYR:N	2.84	0.45
1:A:116:ARG:HG3	1:A:116:ARG:HH21	1.82	0.45
1:A:427:VAL:CG1	1:A:428:GLN:N	2.80	0.45
1:B:1025:PHE:CZ	1:B:1070:VAL:HG11	2.52	0.45
1:A:223:ILE:C	1:A:225:GLN:N	2.67	0.45
1:A:355:VAL:HG13	1:A:356:PRO:CD	2.44	0.45
1:B:1391:ASP:CB	1:B:1420:ARG:HD2	2.46	0.45
1:A:342:ILE:HG22	1:A:343:SER:N	2.32	0.44
1:B:1131:THR:O	1:B:1132:ARG:HG3	2.17	0.44
1:B:1391:ASP:O	1:B:1392:ILE:CG1	2.57	0.44
1:A:365:ARG:CG	1:A:366:SER:H	2.31	0.44
1:B:1121:THR:O	1:B:1124:SER:HB3	2.18	0.44
1:B:1190:PHE:O	1:B:1193:LEU:N	2.50	0.44
1:B:1297:ARG:O	1:B:1301:ILE:HG13	2.16	0.44
1:A:331:ASN:CG	1:A:332:ARG:N	2.65	0.44
1:A:39:ILE:O	1:A:42:ASP:HB2	2.16	0.44
1:B:1043:PHE:CE1	1:B:1052:PHE:CD2	3.05	0.44
1:B:1219:PHE:CZ	1:B:1223:ILE:HD11	2.53	0.44
1:B:1222:ASN:O	1:B:1225:GLN:N	2.49	0.44
1:B:1240:LEU:HD12	1:B:1240:LEU:N	2.32	0.44
1:A:209:ALA:O	1:A:395:PHE:HA	2.18	0.44
1:A:289:TYR:CD1	1:A:289:TYR:N	2.86	0.44
1:B:1386:ILE:CD1	1:B:1393:VAL:HG11	2.47	0.44
1:A:327:GLY:HA3	1:A:338:GLU:CD	2.38	0.44
1:A:66:ASP:OD2	1:A:69:THR:HG23	2.18	0.44
1:B:1025:PHE:CZ	1:B:1089:LEU:HD22	2.53	0.44
1:B:1320:ASP:HA	1:B:1360:LEU:HD12	2.00	0.44
1:B:1068:VAL:O	1:B:1070:VAL:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1231:THR:HG21	1:B:1233:GLU:HG2	1.98	0.44
1:B:1309:LYS:O	1:B:1309:LYS:HG2	2.18	0.44
1:A:391:ASP:O	1:A:419:GLN:HA	2.18	0.44
1:A:50:LYS:HG2	1:A:79:GLN:NE2	2.32	0.44
1:B:1121:THR:CG2	1:B:1147:ILE:HD13	2.48	0.44
1:B:1292:ASP:O	1:B:1292:ASP:CG	2.56	0.44
1:A:260:ALA:HA	1:A:263:LEU:HB3	2.00	0.44
1:B:1186:ILE:HD12	1:B:1200:PHE:O	2.18	0.44
1:B:1272:ASP:HA	1:B:1275:LYS:CG	2.47	0.44
1:B:1053:HIS:O	1:B:1057:ARG:N	2.44	0.44
1:B:1272:ASP:CA	1:B:1275:LYS:HG2	2.46	0.44
1:B:1322:LEU:C	1:B:1324:LEU:N	2.71	0.44
1:A:193:LEU:HA	1:A:427:VAL:CG2	2.47	0.43
1:A:214:VAL:HG12	1:A:214:VAL:O	2.19	0.43
1:A:321:TYR:HA	1:A:360:LEU:O	2.18	0.43
1:A:74:LEU:HD21	1:A:83:VAL:CG2	2.45	0.43
1:B:1050:LYS:O	1:B:1053:HIS:HB3	2.17	0.43
1:B:1126:ALA:C	1:B:1128:ASP:N	2.70	0.43
1:A:161:ASN:ND2	1:A:163:LYS:HB3	2.33	0.43
1:A:358:ILE:CG1	1:A:358:ILE:O	2.53	0.43
1:B:1206:ILE:HG22	1:B:1207:ILE:N	2.33	0.43
1:B:1137:ASP:HB3	1:B:1297:ARG:NH2	2.32	0.43
1:A:293:THR:HG21	1:A:296:ILE:HG12	2.00	0.43
1:B:1246:GLN:O	1:B:1250:ARG:HB2	2.18	0.43
1:A:186:ILE:HA	1:A:187:PRO:HD2	1.87	0.43
1:A:114:LEU:C	1:A:114:LEU:HD13	2.39	0.43
1:B:1182:ASP:O	1:B:1183:ILE:HG22	2.18	0.43
1:B:1209:ALA:HB3	1:B:1395:PHE:CE1	2.54	0.43
1:A:191:THR:N	1:A:440:ASN:HD21	2.17	0.43
1:B:1055:MET:O	1:B:1058:VAL:HG22	2.19	0.43
1:B:1187:PRO:C	1:B:1189:GLY:N	2.71	0.43
1:B:1296:ILE:HG12	1:B:1297:ARG:H	1.84	0.43
1:A:99:ALA:O	1:A:101:ASN:N	2.52	0.43
1:A:432:ILE:HD11	1:A:439:VAL:HG21	2.01	0.43
1:A:190:PHE:HA	1:A:440:ASN:HD21	1.83	0.43
1:B:1275:LYS:HG3	1:B:1276:LEU:N	2.33	0.43
1:B:1333:GLU:HG2	1:B:1333:GLU:H	1.57	0.43
1:A:308:LEU:O	1:A:309:LYS:C	2.56	0.43
1:A:209:ALA:HB2	1:A:361:SER:HB3	2.01	0.43
1:B:1045:ARG:CD	1:B:1046:ALA:H	2.32	0.43
1:B:1386:ILE:HG13	1:B:1387:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASN:HD22	1:A:222:ASN:N	2.16	0.43
1:A:237:ILE:HG21	1:A:247:LEU:HD11	2.01	0.43
1:A:263:LEU:CA	1:A:268:LEU:HD21	2.47	0.43
1:A:363:LEU:CD2	1:A:367:VAL:HG13	2.28	0.43
1:B:1391:ASP:CB	1:B:1420:ARG:CG	2.93	0.43
2:C:2003:DT:C2'	2:C:2004:DT:OP2	2.66	0.43
1:A:104:TYR:O	1:A:105:TYR:C	2.57	0.42
1:A:214:VAL:O	1:A:216:LYS:N	2.52	0.42
1:A:283:LEU:O	1:A:286:ALA:HB3	2.19	0.42
1:A:321:TYR:CE2	1:A:324:LEU:CD1	2.84	0.42
1:B:1024:VAL:O	1:B:1025:PHE:C	2.57	0.42
1:B:1056:LEU:HA	1:B:1056:LEU:HD22	1.84	0.42
1:B:1102:VAL:CG1	1:B:1103:GLU:N	2.81	0.42
1:B:1302:ARG:CB	1:B:1349:LEU:HD13	2.48	0.42
1:B:1346:LEU:O	1:B:1349:LEU:N	2.51	0.42
1:A:103:GLU:O	1:A:104:TYR:C	2.57	0.42
1:A:220:ALA:HB2	1:A:360:LEU:CD2	2.47	0.42
1:A:418:LYS:CG	1:A:419:GLN:N	2.81	0.42
1:A:73:GLU:O	1:A:76:ALA:HB3	2.18	0.42
1:A:183:ILE:HG23	1:A:199:GLY:HA3	2.00	0.42
1:B:1052:PHE:O	1:B:1055:MET:CB	2.68	0.42
1:B:1054:ALA:CB	1:B:1074:LEU:HD11	2.49	0.42
1:B:1251:MET:SD	1:B:1288:ILE:CD1	3.07	0.42
1:A:267:LYS:O	1:A:267:LYS:HG2	2.19	0.42
1:A:283:LEU:C	1:A:286:ALA:H	2.21	0.42
1:A:96:VAL:HG22	1:A:98:THR:N	2.35	0.42
1:B:1340:SER:C	1:B:1342:ILE:N	2.70	0.42
1:A:237:ILE:HA	1:A:318:VAL:CG1	2.47	0.42
1:A:269:THR:N	1:A:272:ASP:HB2	2.35	0.42
1:B:1025:PHE:HZ	1:B:1089:LEU:HD22	1.84	0.42
1:B:1392:ILE:HG22	1:B:1392:ILE:O	2.18	0.42
1:A:259:ASN:O	1:A:261:GLN:N	2.53	0.42
1:A:227:VAL:HG13	1:A:231:THR:CG2	2.47	0.42
1:A:9:ILE:HG13	1:A:9:ILE:O	2.19	0.42
1:B:1033:LEU:HD22	1:B:1033:LEU:HA	1.73	0.42
1:B:1110:GLU:O	1:B:1111:GLU:C	2.57	0.42
1:A:116:ARG:HG3	1:A:116:ARG:NH2	2.34	0.42
1:B:1098:THR:OG1	1:B:1099:ALA:N	2.52	0.42
1:B:1221:LEU:O	1:B:1225:GLN:HG3	2.20	0.42
1:B:1391:ASP:CB	1:B:1420:ARG:CD	2.97	0.42
1:A:167:VAL:CG2	1:A:168:GLN:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:THR:O	1:A:189:GLY:C	2.58	0.42
1:A:202:ARG:O	1:A:203:SER:CB	2.67	0.42
1:A:260:ALA:O	1:A:261:GLN:C	2.58	0.42
1:A:261:GLN:HA	1:A:264:ARG:CZ	2.49	0.42
1:A:302:ARG:NH1	1:A:352:GLU:OE1	2.53	0.42
1:B:1210:ALA:HB1	1:B:1214:VAL:HG11	2.02	0.42
1:B:1126:ALA:O	1:B:1127:GLN:C	2.59	0.42
1:B:1335:ARG:HD3	1:B:1335:ARG:O	2.20	0.42
1:A:295:SER:OG	2:C:2009:DT:H73	2.20	0.42
1:A:66:ASP:OD2	1:A:66:ASP:O	2.38	0.41
1:B:1037:ARG:HH21	1:B:1107:ARG:NH1	2.14	0.41
1:B:1110:GLU:O	1:B:1113:SER:N	2.53	0.41
1:A:101:ASN:HB2	1:A:105:TYR:CZ	2.55	0.41
1:A:50:LYS:HG2	1:A:79:GLN:CD	2.41	0.41
1:B:1191:THR:O	1:B:1195:ARG:N	2.51	0.41
1:A:429:LEU:HD23	1:A:438:PHE:CD2	2.55	0.41
1:A:89:LEU:O	1:A:90:SER:C	2.59	0.41
1:B:1135:GLU:HB2	1:B:1139:LEU:HD12	2.01	0.41
1:B:1208:VAL:HA	1:B:1394:ALA:O	2.21	0.41
1:B:1322:LEU:N	1:B:1322:LEU:HD23	2.35	0.41
1:A:205:LEU:HD21	1:A:346:LEU:CB	2.50	0.41
1:A:197:THR:O	1:A:198:SER:HB2	2.20	0.41
1:A:214:VAL:CG1	1:A:217:THR:OG1	2.68	0.41
1:A:214:VAL:HG12	1:A:217:THR:HB	2.01	0.41
1:B:1088:TYR:HA	1:B:1091:GLU:HG3	2.03	0.41
1:B:1142:GLU:HA	1:B:1145:ARG:HB3	2.02	0.41
1:B:1342:ILE:O	1:B:1346:LEU:N	2.50	0.41
1:B:1012:GLN:HG3	1:B:1012:GLN:O	2.21	0.41
1:B:1271:GLU:HG2	1:B:1275:LYS:HZ2	1.85	0.41
1:B:1073:GLU:OE1	1:B:1073:GLU:HA	2.21	0.41
1:B:1190:PHE:O	1:B:1192:GLU:N	2.53	0.41
1:B:1245:GLN:O	1:B:1246:GLN:C	2.59	0.41
1:B:1290:ILE:CG2	1:B:1291:ASP:H	2.30	0.41
1:B:1317:VAL:HG13	1:B:1317:VAL:O	2.20	0.41
1:A:347:LYS:HB2	1:A:389:ASP:HB3	2.02	0.41
1:B:1101:ASN:ND2	1:B:1102:VAL:H	2.12	0.41
1:B:1131:THR:O	1:B:1132:ARG:CG	2.69	0.41
1:B:1221:LEU:O	1:B:1222:ASN:C	2.59	0.41
1:B:1234:ASN:N	1:B:1234:ASN:ND2	2.68	0.41
1:B:1242:MET:HB3	1:B:1242:MET:HE2	1.83	0.41
1:A:237:ILE:HG12	1:A:318:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:O	1:A:70:VAL:CG1	2.69	0.41
1:A:18:GLN:HG3	1:A:95:SER:CB	2.52	0.41
1:A:406:SER:O	1:A:407:GLU:HB2	2.19	0.41
1:A:342:ILE:O	1:A:343:SER:C	2.58	0.40
1:B:1026:LEU:HD23	1:B:1098:THR:C	2.41	0.40
1:B:1170:TYR:O	1:B:1173:ILE:CG2	2.68	0.40
1:A:26:LEU:HD23	1:A:26:LEU:N	2.35	0.40
1:A:375:PRO:HD2	1:A:397:TYR:HB2	2.03	0.40
1:A:40:PRO:HG3	1:A:52:PHE:CD2	2.45	0.40
1:A:439:VAL:HG12	1:A:440:ASN:N	2.36	0.40
1:B:1330:ARG:O	1:B:1331:ASN:HB2	2.21	0.40
1:B:1344:ARG:NH1	2:C:2009:DT:O2	2.54	0.40
1:A:101:ASN:HB2	1:A:105:TYR:OH	2.20	0.40
1:A:278:MET:O	1:A:279:ALA:C	2.59	0.40
1:A:338:GLU:O	1:A:341:GLU:HG2	2.21	0.40
1:B:1037:ARG:O	1:B:1038:LEU:HD23	2.20	0.40
1:B:1021:LEU:HG	1:B:1043:PHE:HE2	1.85	0.40
1:B:1200:PHE:CD2	1:B:1206:ILE:HG12	2.57	0.40
1:A:37:ARG:HG3	1:A:110:GLU:OE1	2.21	0.40
1:B:1111:GLU:O	1:B:1112:LYS:C	2.59	0.40
1:B:1132:ARG:HB2	1:B:1139:LEU:HD11	2.02	0.40
1:B:1104:TYR:O	1:B:1107:ARG:HB2	2.21	0.40
1:B:1108:ILE:O	1:B:1109:VAL:C	2.60	0.40
1:B:1115:LEU:HD23	1:B:1115:LEU:HA	1.64	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	417/454 (92%)	323 (78%)	75 (18%)	19 (5%)	<b>2</b> <b>23</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	369/454 (81%)	268 (73%)	75 (20%)	26 (7%)	1	16
All	All	786/908 (87%)	591 (75%)	150 (19%)	45 (6%)	1	20

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	321	TYR
1	B	1126	ALA
1	B	1321	TYR
1	B	1334	ASN
1	B	1392	ILE
1	A	189	GLY
1	A	212	PRO
1	A	329	GLY
1	A	406	SER
1	B	1067	LEU
1	B	1069	THR
1	B	1127	GLN
1	B	1382	GLU
1	A	83	VAL
1	A	100	ALA
1	A	135	GLU
1	A	214	VAL
1	B	1009	ILE
1	B	1055	MET
1	B	1059	ALA
1	B	1133	GLU
1	B	1191	THR
1	B	1222	ASN
1	B	1294	PRO
1	B	1326	GLN
1	A	78	GLU
1	A	244	ALA
1	B	1031	LEU
1	B	1138	VAL
1	A	55	MET
1	A	365	ARG
1	B	1325	ILE
1	A	15	GLU
1	A	315	GLY
1	B	1102	VAL

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Mol	Chain	Res	Type
1	B	1389	ASP
1	B	1183	ILE
1	B	1223	ILE
1	B	1313	GLY
1	A	40	PRO
1	B	1010	PRO
1	A	215	GLY
1	A	97	PRO
1	B	1068	VAL

### 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	361/388 (93%)	311 (86%)	50 (14%)	3	20
1	B	320/388 (82%)	272 (85%)	48 (15%)	3	17
All	All	681/776 (88%)	583 (86%)	98 (14%)	3	18

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	37	ARG
1	A	38	LEU
1	A	41	GLU
1	A	53	HIS
1	A	57	ARG
1	A	63	GLU
1	A	74	LEU
1	A	77	LEU
1	A	95	SER
1	A	98	THR
1	A	133	GLU
1	A	159	PHE
1	A	170	TYR

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Mol	Chain	Res	Type
1	A	173	ILE
1	A	175	MET
1	A	192	GLU
1	A	200	PHE
1	A	204	ASP
1	A	216	LYS
1	A	229	THR
1	A	231	THR
1	A	233	GLU
1	A	249	MET
1	A	252	LEU
1	A	262	ASN
1	A	272	ASP
1	A	277	THR
1	A	290	ILE
1	A	296	ILE
1	A	310	GLN
1	A	316	MET
1	A	322	LEU
1	A	330	ARG
1	A	331	ASN
1	A	332	ARG
1	A	333	GLU
1	A	336	GLN
1	A	342	ILE
1	A	349	LEU
1	A	351	ARG
1	A	360	LEU
1	A	362	GLN
1	A	365	ARG
1	A	371	GLN
1	A	380	LEU
1	A	385	SER
1	A	388	GLN
1	A	412	ILE
1	A	434	GLU
1	B	1007	GLU
1	B	1033	LEU
1	B	1039	ILE
1	B	1055	MET
1	B	1056	LEU
1	B	1101	ASN

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Mol	Chain	Res	Type
1	B	1103	GLU
1	B	1115	LEU
1	B	1116	ARG
1	B	1121	THR
1	B	1134	ASP
1	B	1137	ASP
1	B	1139	LEU
1	B	1141	ASP
1	B	1165	VAL
1	B	1171	ASP
1	B	1172	ASN
1	B	1175	MET
1	B	1176	LEU
1	B	1178	ASN
1	B	1198	SER
1	B	1204	ASP
1	B	1213	SER
1	B	1221	LEU
1	B	1226	ASN
1	B	1250	ARG
1	B	1253	CYS
1	B	1276	LEU
1	B	1278	MET
1	B	1280	MET
1	B	1316	MET
1	B	1321	TYR
1	B	1323	GLN
1	B	1331	ASN
1	B	1332	ARG
1	B	1333	GLU
1	B	1338	GLU
1	B	1365	ARG
1	B	1370	ARG
1	B	1374	ARG
1	B	1379	ASP
1	B	1385	SER
1	B	1386	ILE
1	B	1387	GLU
1	B	1389	ASP
1	B	1391	ASP
1	B	1393	VAL
1	B	1415	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	168	GLN
1	A	226	ASN
1	A	232	ASN
1	A	246	GLN
1	A	259	ASN
1	A	261	GLN
1	A	262	ASN
1	A	323	GLN
1	A	326	GLN
1	A	331	ASN
1	A	336	GLN
1	A	371	GLN
1	A	388	GLN
1	A	403	ASN
1	A	408	ASN
1	A	419	GLN
1	A	428	GLN
1	A	440	ASN
1	B	1053	HIS
1	B	1101	ASN
1	B	1178	ASN
1	B	1222	ASN
1	B	1225	GLN
1	B	1234	ASN
1	B	1331	ASN
1	B	1362	GLN
1	B	1419	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	425/454 (93%)	0.06	7 (1%) 72 62	54, 165, 267, 298	0
1	B	381/454 (83%)	0.14	15 (3%) 39 31	58, 191, 280, 298	0
2	C	9/9 (100%)	-0.30	0 100 100	255, 293, 298, 298	0
All	All	815/917 (88%)	0.10	22 (2%) 54 44	54, 177, 279, 298	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1395	PHE	4.5
1	B	1380	LEU	3.9
1	B	1316	MET	3.7
1	B	1043	PHE	3.2
1	B	1357	VAL	3.1
1	B	1358	ILE	3.0
1	B	1359	ALA	2.9
1	A	159	PHE	2.8
1	A	428	GLN	2.8
1	B	1317	VAL	2.7
1	B	1184	THR	2.6
1	B	1296	ILE	2.6
1	B	1200	PHE	2.6
1	A	316	MET	2.6
1	B	1322	LEU	2.5
1	A	160	LYS	2.5
1	A	322	LEU	2.5
1	B	1268	LEU	2.3
1	A	251	MET	2.3
1	B	1037	ARG	2.3
1	A	125	ILE	2.2
1	B	1295	SER	2.2

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.