



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:05 PM GMT

PDB ID : 2R6D  
Title : Crystal Form B1  
Authors : Bailey, S.; Eliason, W.K.; Steitz, T.A.  
Deposited on : 2007-09-05  
Resolution : 3.70 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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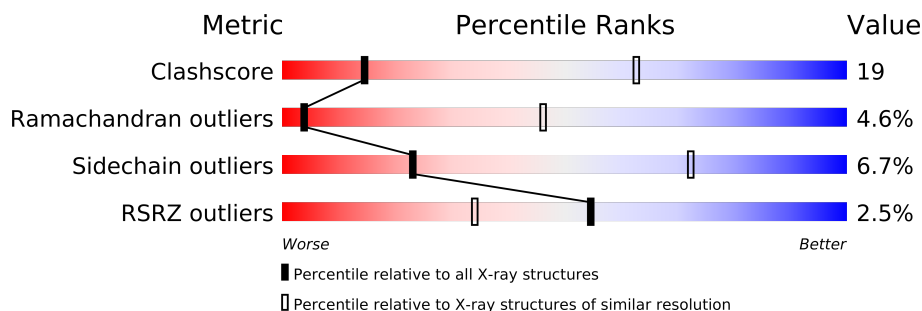
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.70 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))
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	454	
1	B	454	
1	C	454	
1	D	454	
1	E	454	
1	F	454	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18085 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

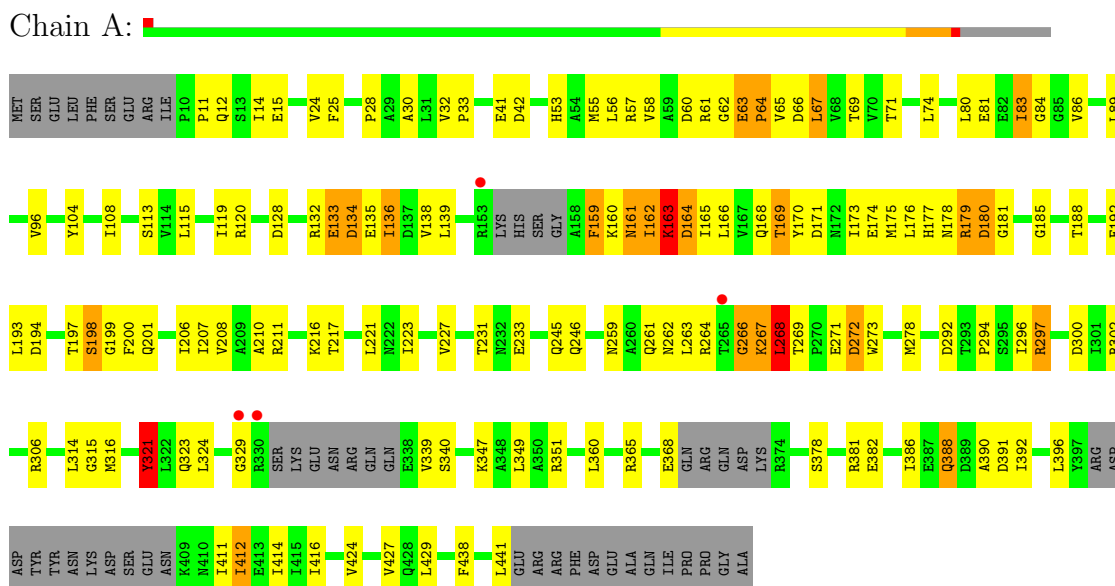
- Molecule 1 is a protein called Replicative helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3138	1969	544	611	14			
1	B	376	Total	C	N	O	S	0	0	0
			2897	1820	500	564	13			
1	C	399	Total	C	N	O	S	0	0	0
			3089	1938	534	603	14			
1	D	376	Total	C	N	O	S	0	0	0
			2897	1820	500	564	13			
1	E	392	Total	C	N	O	S	0	0	0
			3032	1905	521	593	13			
1	F	392	Total	C	N	O	S	0	0	0
			3032	1905	521	593	13			

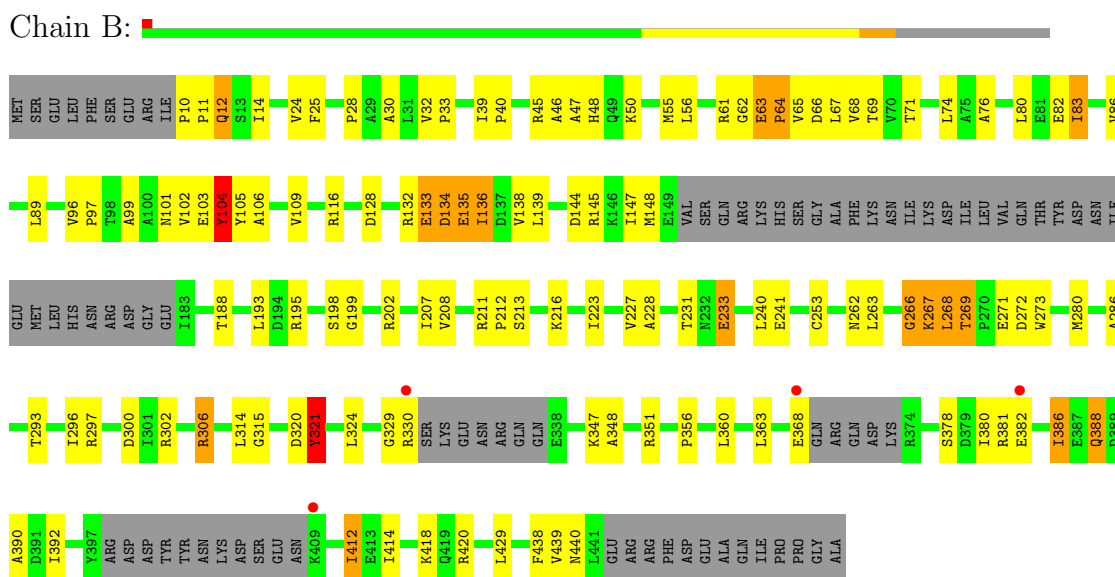
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Replicative helicase



#### • Molecule 1: Replicative helicase

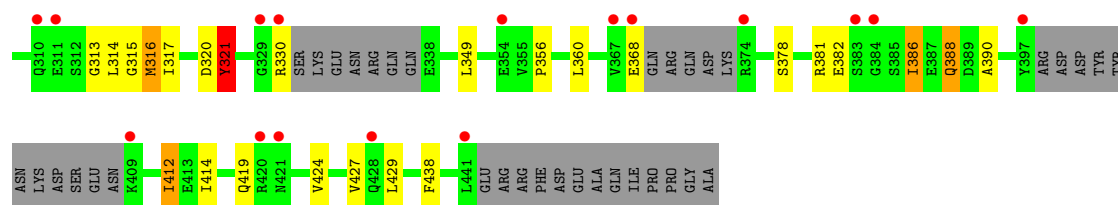


#### • Molecule 1: Replicative helicase



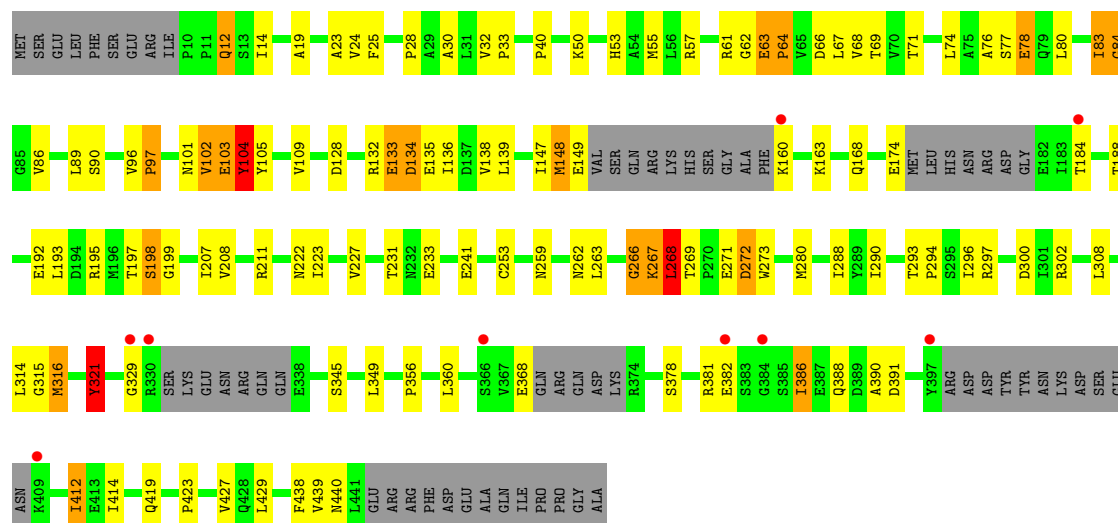
Government	Percentage
Current government	100%
Previous government	0%





### ● Molecule 1: Replicative helicase

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	371.26Å 110.30Å 112.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 19.99 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-3.70) 98.0 (19.99-3.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.71Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.309 , 0.322 0.292 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	145.4	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 196.5	EDS
Estimated twinning fraction	0.077 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 49014 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.45	0/3173	0.68	1/4285 (0.0%)
1	B	0.46	0/2929	0.72	1/3957 (0.0%)
1	C	0.47	1/3123 (0.0%)	0.70	4/4218 (0.1%)
1	D	0.41	0/2929	0.69	3/3957 (0.1%)
1	E	0.38	0/3064	0.64	0/4138
1	F	0.41	0/3064	0.69	2/4138 (0.0%)
All	All	0.43	1/18282 (0.0%)	0.69	11/24693 (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	B	1	0
1	C	1	2
1	D	1	1
1	E	1	0
1	F	1	1
All	All	5	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	GLU	CD-OE2	6.40	1.32	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	GLY	N-CA-C	-6.08	97.91	113.10
1	C	174	GLU	O-C-N	5.89	132.12	122.70
1	A	321	TYR	N-CA-C	5.85	126.79	111.00
1	B	321	TYR	N-CA-C	5.79	126.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	TYR	N-CA-C	5.68	126.34	111.00
1	F	321	TYR	N-CA-C	5.50	125.85	111.00
1	C	103	GLU	N-CA-C	5.34	125.42	111.00
1	D	321	TYR	N-CA-C	5.19	125.00	111.00
1	F	84	GLY	N-CA-C	-5.13	100.26	113.10
1	D	103	GLU	C-N-CA	5.04	134.30	121.70
1	D	133	GLU	C-N-CA	5.02	134.25	121.70

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	104	TYR	CA
1	C	104	TYR	CA
1	D	104	TYR	CA
1	E	104	TYR	CA
1	F	104	TYR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	103	GLU	Peptide
1	C	174	GLU	Mainchain
1	D	104	TYR	Peptide
1	F	104	TYR	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3138	0	3190	134	0
1	B	2897	0	2953	131	0
1	C	3089	0	3141	148	2
1	D	2897	0	2953	154	0
1	E	3032	0	3087	115	0
1	F	3032	0	3087	108	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18085	0	18411	705	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (705) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:133:GLU:N	1:A:134:ASP:HB2	1.33	1.43
1:E:133:GLU:N	1:E:134:ASP:HB2	1.36	1.40
1:F:133:GLU:N	1:F:134:ASP:HB2	1.39	1.38
1:C:133:GLU:N	1:C:134:ASP:HB2	1.32	1.35
1:E:330:ARG:NH1	1:F:148:MET:O	1.63	1.32
1:C:133:GLU:H	1:C:134:ASP:CB	1.43	1.30
1:B:133:GLU:N	1:B:134:ASP:HB2	1.42	1.30
1:A:133:GLU:H	1:A:134:ASP:CB	1.45	1.27
1:D:133:GLU:N	1:D:134:ASP:HB2	1.47	1.26
1:E:133:GLU:H	1:E:134:ASP:CB	1.48	1.23
1:D:133:GLU:H	1:D:134:ASP:CB	1.51	1.22
1:C:174:GLU:O	1:C:177:HIS:N	1.73	1.22
1:C:294:PRO:HB2	1:D:381:ARG:NE	1.58	1.18
1:F:133:GLU:H	1:F:134:ASP:CB	1.57	1.17
1:B:133:GLU:H	1:B:134:ASP:CB	1.62	1.13
1:D:62:GLY:HA2	1:D:63:GLU:HB3	1.31	1.11
1:F:63:GLU:H	1:F:64:PRO:HA	1.14	1.10
1:D:63:GLU:H	1:D:64:PRO:HA	1.12	1.07
1:C:104:TYR:HB3	1:C:105:TYR:HB2	1.34	1.06
1:D:135:GLU:HG2	1:D:330:ARG:HH21	1.16	1.05
1:B:133:GLU:H	1:B:134:ASP:HB2	0.91	1.03
1:B:268:LEU:HB2	1:C:177:HIS:HE1	1.19	1.03
1:D:133:GLU:H	1:D:134:ASP:HB2	0.87	1.02
1:E:104:TYR:HA	1:E:105:TYR:HB2	1.38	1.01
1:E:61:ARG:HB2	1:E:62:GLY:HA3	1.39	1.01
1:A:294:PRO:HG3	1:B:348:ALA:HA	1.40	0.99
1:D:135:GLU:HG2	1:D:330:ARG:NH2	1.78	0.99
1:E:330:ARG:CZ	1:F:148:MET:O	2.10	0.99
1:F:61:ARG:HB2	1:F:62:GLY:HA3	1.44	0.98
1:E:19:ALA:HA	1:E:96:VAL:HG21	1.44	0.97
1:C:61:ARG:HB2	1:C:62:GLY:HA3	1.44	0.96
1:B:104:TYR:HB3	1:B:105:TYR:HB2	1.44	0.96
1:A:306:ARG:NH2	1:B:103:GLU:OE2	1.99	0.96
1:E:63:GLU:H	1:E:64:PRO:HA	1.27	0.96
1:F:207:ILE:HD12	1:F:390:ALA:HB2	1.48	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:61:ARG:HB2	1:D:62:GLY:HA3	1.50	0.94
1:A:61:ARG:CB	1:A:62:GLY:HA3	1.98	0.93
1:E:207:ILE:HD12	1:E:390:ALA:HB2	1.50	0.92
1:C:294:PRO:HB2	1:D:381:ARG:CD	1.98	0.92
1:D:145:ARG:NH1	1:D:328:SER:H	1.66	0.92
1:D:145:ARG:HD3	1:D:328:SER:OG	1.70	0.91
1:C:171:ASP:O	1:C:175:MET:HG3	1.70	0.91
1:D:145:ARG:HG3	1:D:341:GLU:OE1	1.70	0.91
1:D:145:ARG:HH11	1:D:328:SER:H	0.93	0.91
1:C:61:ARG:CB	1:C:62:GLY:HA3	2.00	0.90
1:E:104:TYR:CA	1:E:105:TYR:HB2	2.03	0.89
1:A:207:ILE:HD12	1:A:390:ALA:HB2	1.51	0.88
1:B:268:LEU:HB2	1:C:177:HIS:CE1	2.09	0.87
1:C:174:GLU:CG	1:C:175:MET:N	2.35	0.87
1:E:330:ARG:HG3	1:F:149:GLU:HG2	1.53	0.87
1:D:104:TYR:HB3	1:D:105:TYR:HB2	1.57	0.86
1:E:265:THR:HG23	1:F:423:PRO:HB3	1.57	0.85
1:F:101:ASN:O	1:F:103:GLU:N	2.07	0.85
1:D:145:ARG:HH11	1:D:328:SER:N	1.73	0.85
1:F:61:ARG:CB	1:F:62:GLY:HA3	2.04	0.84
1:B:63:GLU:H	1:B:64:PRO:HA	1.42	0.84
1:F:32:VAL:HB	1:F:33:PRO:HD3	1.58	0.83
1:F:104:TYR:HB3	1:F:105:TYR:HB2	1.60	0.83
1:E:61:ARG:CB	1:E:62:GLY:HA3	2.08	0.83
1:D:32:VAL:HB	1:D:33:PRO:HD3	1.60	0.83
1:A:227:VAL:O	1:A:231:THR:HG22	1.79	0.83
1:C:294:PRO:HG2	1:D:381:ARG:CZ	2.09	0.83
1:C:174:GLU:OE2	1:C:178:ASN:HB3	1.79	0.83
1:E:104:TYR:HB3	1:E:105:TYR:HB2	1.61	0.82
1:F:67:LEU:O	1:F:71:THR:HG23	1.79	0.82
1:D:265:THR:HG23	1:E:424:VAL:H	1.44	0.81
1:C:207:ILE:HD13	1:C:386:ILE:HG22	1.62	0.81
1:D:135:GLU:CG	1:D:330:ARG:HH21	1.92	0.81
1:D:142:GLU:N	1:D:328:SER:HB2	1.95	0.81
1:F:302:ARG:HG2	1:F:349:LEU:HD13	1.63	0.81
1:A:198:SER:N	1:A:199:GLY:HA2	1.96	0.80
1:D:63:GLU:N	1:D:64:PRO:HA	1.96	0.80
1:D:19:ALA:HA	1:D:96:VAL:HG21	1.62	0.80
1:A:246:GLN:NE2	1:B:420:ARG:HB3	1.97	0.80
1:A:294:PRO:HG3	1:B:348:ALA:CA	2.11	0.79
1:D:62:GLY:HA2	1:D:63:GLU:CB	1.99	0.79
1:D:145:ARG:NH1	1:D:328:SER:N	2.30	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:198:SER:N	1:F:199:GLY:HA2	1.97	0.79
1:C:172:ASN:HA	1:C:175:MET:HB2	1.64	0.79
1:F:63:GLU:N	1:F:64:PRO:HA	1.96	0.79
1:C:175:MET:O	1:C:179:ARG:HD2	1.83	0.79
1:D:101:ASN:O	1:D:103:GLU:N	2.15	0.79
1:E:198:SER:N	1:E:199:GLY:HA2	1.98	0.78
1:C:198:SER:N	1:C:199:GLY:HA2	1.98	0.78
1:A:188:THR:HG21	1:A:193:LEU:HD23	1.65	0.78
1:E:32:VAL:HB	1:E:33:PRO:HD3	1.65	0.78
1:E:104:TYR:CB	1:E:105:TYR:HB2	2.13	0.78
1:B:347:LYS:HE3	1:B:351:ARG:CZ	2.14	0.78
1:E:207:ILE:HD13	1:E:386:ILE:HG22	1.67	0.77
1:C:104:TYR:CB	1:C:105:TYR:HB2	2.13	0.76
1:B:61:ARG:HB2	1:B:62:GLY:HA3	1.67	0.76
1:B:268:LEU:HD12	1:C:177:HIS:CE1	2.20	0.76
1:B:267:LYS:O	1:C:177:HIS:CE1	2.40	0.75
1:D:63:GLU:H	1:D:64:PRO:CA	1.98	0.75
1:A:161:ASN:HD21	1:A:163:LYS:HG2	1.52	0.75
1:D:62:GLY:CA	1:D:63:GLU:HB3	2.15	0.75
1:C:306:ARG:HD3	1:D:32:VAL:HG13	1.69	0.75
1:A:61:ARG:HB3	1:A:62:GLY:HA3	1.67	0.75
1:C:294:PRO:CB	1:D:381:ARG:NE	2.46	0.74
1:A:161:ASN:ND2	1:A:163:LYS:HG2	2.02	0.74
1:B:207:ILE:HD12	1:B:390:ALA:HB2	1.68	0.74
1:A:63:GLU:H	1:A:64:PRO:HA	1.52	0.74
1:C:241:GLU:HG3	1:D:378:SER:HB3	1.68	0.74
1:B:198:SER:N	1:B:199:GLY:HA2	2.01	0.74
1:E:66:ASP:H	1:E:69:THR:HG22	1.52	0.74
1:A:381:ARG:HH22	1:A:388:GLN:HE22	1.36	0.74
1:F:207:ILE:HD13	1:F:386:ILE:HG22	1.70	0.73
1:B:61:ARG:CB	1:B:62:GLY:HA3	2.18	0.73
1:B:67:LEU:O	1:B:71:THR:HG23	1.88	0.73
1:D:273:TRP:CH2	1:E:173:ILE:HG22	2.24	0.72
1:D:198:SER:N	1:D:199:GLY:HA2	2.03	0.72
1:C:63:GLU:H	1:C:64:PRO:HA	1.55	0.72
1:F:297:ARG:NH2	1:F:329:GLY:O	2.20	0.72
1:C:207:ILE:HD12	1:C:390:ALA:HB2	1.71	0.71
1:D:145:ARG:CG	1:D:341:GLU:OE1	2.39	0.71
1:A:245:GLN:HE22	1:B:202:ARG:HH12	1.39	0.70
1:F:269:THR:HB	1:F:272:ASP:HB2	1.72	0.70
1:C:28:PRO:C	1:C:30:ALA:H	1.95	0.70
1:C:175:MET:O	1:C:179:ARG:CD	2.39	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:148:MET:HE3	1:C:148:MET:HA	1.73	0.70
1:D:66:ASP:H	1:D:69:THR:HG22	1.55	0.69
1:D:40:PRO:O	1:D:49:GLN:HG2	1.92	0.69
1:F:64:PRO:O	1:F:69:THR:HG21	1.92	0.69
1:D:32:VAL:HG12	1:D:36:GLU:OE1	1.93	0.69
1:C:40:PRO:O	1:C:49:GLN:HG3	1.92	0.69
1:A:159:PHE:HD1	1:A:160:LYS:H	1.40	0.69
1:D:136:ILE:HD12	1:E:115:LEU:HG	1.74	0.69
1:E:63:GLU:N	1:E:64:PRO:HA	2.06	0.69
1:C:241:GLU:O	1:D:377:MET:HB2	1.93	0.68
1:B:207:ILE:HD13	1:B:386:ILE:HG22	1.74	0.68
1:D:66:ASP:H	1:D:69:THR:CG2	2.07	0.68
1:D:61:ARG:CB	1:D:62:GLY:HA3	2.15	0.68
1:C:294:PRO:HG2	1:D:381:ARG:NH2	2.09	0.68
1:A:61:ARG:HB2	1:A:62:GLY:HA3	1.72	0.68
1:C:148:MET:CE	1:C:148:MET:HA	2.22	0.68
1:D:67:LEU:O	1:D:71:THR:HG23	1.94	0.67
1:A:269:THR:HB	1:A:272:ASP:HB2	1.76	0.67
1:E:330:ARG:NH2	1:F:149:GLU:HA	2.09	0.67
1:C:306:ARG:HD3	1:D:32:VAL:CG1	2.25	0.67
1:A:197:THR:O	1:A:198:SER:HB2	1.94	0.67
1:D:290:ILE:O	1:E:160:LYS:HB3	1.94	0.67
1:C:307:ARG:NH2	1:D:36:GLU:OE2	2.27	0.67
1:C:19:ALA:HA	1:C:96:VAL:HG21	1.74	0.67
1:C:175:MET:HB3	1:C:423:PRO:HB3	1.77	0.67
1:D:227:VAL:O	1:D:231:THR:HG22	1.95	0.66
1:C:320:ASP:HA	1:C:360:LEU:HD12	1.76	0.66
1:C:227:VAL:O	1:C:231:THR:HG22	1.95	0.66
1:A:294:PRO:HA	1:B:351:ARG:NH1	2.10	0.66
1:A:65:VAL:HA	1:A:69:THR:HG21	1.78	0.66
1:D:302:ARG:HG2	1:D:349:LEU:HD13	1.78	0.66
1:F:412:ILE:HG21	1:F:438:PHE:HE2	1.62	0.65
1:C:174:GLU:HG3	1:C:175:MET:H	1.62	0.65
1:B:211:ARG:HH11	1:B:368:GLU:HG3	1.60	0.65
1:C:63:GLU:N	1:C:64:PRO:HA	2.11	0.65
1:A:133:GLU:CA	1:A:134:ASP:HB2	2.23	0.65
1:B:253:CYS:SG	1:B:263:LEU:HD12	2.37	0.65
1:C:174:GLU:HG3	1:C:175:MET:N	2.11	0.65
1:E:188:THR:HG21	1:E:193:LEU:HD23	1.77	0.65
1:C:211:ARG:HH11	1:C:368:GLU:HG3	1.62	0.65
1:F:23:ALA:HB1	1:F:102:VAL:HG22	1.79	0.65
1:C:132:ARG:O	1:C:133:GLU:HG3	1.96	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:330:ARG:HG3	1:F:149:GLU:CG	2.24	0.64
1:C:294:PRO:CG	1:D:381:ARG:CZ	2.75	0.64
1:A:211:ARG:HH11	1:A:368:GLU:HG3	1.62	0.64
1:D:269:THR:HB	1:D:272:ASP:HB2	1.79	0.64
1:B:227:VAL:O	1:B:231:THR:HG22	1.98	0.64
1:E:23:ALA:HB1	1:E:102:VAL:HG22	1.80	0.64
1:A:66:ASP:H	1:A:69:THR:HG22	1.63	0.64
1:F:211:ARG:HH11	1:F:368:GLU:HG3	1.63	0.64
1:B:104:TYR:CB	1:B:105:TYR:HB2	2.22	0.64
1:C:12:GLN:HE21	1:C:14:ILE:HG12	1.63	0.64
1:A:173:ILE:HD12	1:F:263:LEU:HD22	1.80	0.64
1:F:227:VAL:O	1:F:231:THR:HG22	1.98	0.64
1:F:63:GLU:H	1:F:64:PRO:CA	2.02	0.63
1:E:104:TYR:HA	1:E:105:TYR:CB	2.19	0.63
1:E:63:GLU:H	1:E:64:PRO:CA	2.05	0.63
1:D:207:ILE:HD12	1:D:390:ALA:HB2	1.80	0.63
1:A:266:GLY:HA2	1:A:267:LYS:O	1.98	0.63
1:D:41:GLU:HA	1:D:49:GLN:HE21	1.64	0.63
1:C:381:ARG:HH22	1:C:388:GLN:HE22	1.47	0.63
1:B:74:LEU:HD13	1:B:83:ILE:CD1	2.28	0.63
1:E:62:GLY:HA2	1:E:63:GLU:HB3	1.79	0.62
1:A:174:GLU:OE1	1:A:178:ASN:HB2	1.97	0.62
1:E:101:ASN:O	1:E:103:GLU:N	2.33	0.62
1:C:307:ARG:HE	1:D:36:GLU:CD	2.02	0.62
1:A:171:ASP:O	1:A:174:GLU:HG3	1.99	0.62
1:E:65:VAL:HA	1:E:69:THR:HG21	1.81	0.62
1:C:207:ILE:HD13	1:C:386:ILE:CG2	2.28	0.62
1:E:381:ARG:HH22	1:E:388:GLN:HE22	1.46	0.62
1:E:227:VAL:O	1:E:231:THR:HG22	2.00	0.62
1:A:71:THR:HG22	1:A:89:LEU:HD13	1.82	0.62
1:D:133:GLU:CA	1:D:134:ASP:HB2	2.30	0.62
1:C:147:ILE:HG22	1:C:147:ILE:O	1.98	0.62
1:D:188:THR:HG21	1:D:193:LEU:HD23	1.81	0.61
1:A:133:GLU:H	1:A:134:ASP:HB2	0.55	0.61
1:C:23:ALA:HB1	1:C:102:VAL:HG22	1.83	0.61
1:F:62:GLY:HA2	1:F:63:GLU:HB3	1.82	0.61
1:E:19:ALA:O	1:E:23:ALA:HB2	2.00	0.61
1:E:47:ALA:HB1	1:E:83:ILE:HG23	1.82	0.61
1:C:147:ILE:CG2	1:C:147:ILE:O	2.48	0.61
1:D:296:ILE:CG2	1:D:300:ASP:HB2	2.31	0.61
1:A:296:ILE:CG2	1:A:300:ASP:HB2	2.30	0.61
1:F:267:LYS:O	1:F:268:LEU:HB2	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:VAL:HB	1:A:33:PRO:HD3	1.82	0.60
1:B:39:ILE:HB	1:B:40:PRO:HD2	1.84	0.60
1:C:296:ILE:HG22	1:C:300:ASP:HB2	1.83	0.60
1:A:198:SER:H	1:A:199:GLY:HA2	1.66	0.60
1:A:296:ILE:HG22	1:A:300:ASP:HB2	1.83	0.60
1:C:174:GLU:C	1:C:176:LEU:N	2.54	0.60
1:D:141:ASP:C	1:D:143:ALA:H	2.04	0.60
1:A:162:ILE:O	1:A:164:ASP:N	2.35	0.60
1:D:266:GLY:HA2	1:D:267:LYS:O	2.02	0.60
1:C:133:GLU:CA	1:C:134:ASP:HB2	2.27	0.60
1:C:171:ASP:O	1:C:175:MET:CG	2.48	0.60
1:A:67:LEU:O	1:A:71:THR:HG23	2.02	0.60
1:B:63:GLU:N	1:B:64:PRO:HA	2.14	0.59
1:C:412:ILE:HG21	1:C:438:PHE:CE2	2.37	0.59
1:C:412:ILE:HG21	1:C:438:PHE:HE2	1.66	0.59
1:A:246:GLN:HE22	1:B:420:ARG:HB3	1.65	0.59
1:F:62:GLY:CA	1:F:63:GLU:HB3	2.32	0.59
1:C:294:PRO:CB	1:D:381:ARG:CD	2.78	0.59
1:D:135:GLU:HG2	1:D:330:ARG:CZ	2.32	0.59
1:D:296:ILE:HG22	1:D:300:ASP:HB2	1.82	0.59
1:F:188:THR:HG21	1:F:193:LEU:HD23	1.83	0.59
1:B:50:LYS:NZ	1:B:82:GLU:OE2	2.36	0.59
1:C:103:GLU:N	1:C:104:TYR:HB2	2.17	0.59
1:D:135:GLU:CG	1:D:330:ARG:NH2	2.55	0.59
1:D:62:GLY:CA	1:D:63:GLU:CB	2.76	0.59
1:E:101:ASN:C	1:E:103:GLU:H	2.06	0.58
1:F:296:ILE:CG2	1:F:300:ASP:HB2	2.33	0.58
1:A:61:ARG:CB	1:A:62:GLY:CA	2.79	0.58
1:F:412:ILE:HG21	1:F:438:PHE:CE2	2.38	0.58
1:D:207:ILE:HD13	1:D:386:ILE:HG22	1.83	0.58
1:B:381:ARG:HH22	1:B:388:GLN:HE22	1.51	0.58
1:B:25:PHE:HZ	1:B:89:LEU:HD22	1.68	0.58
1:B:66:ASP:H	1:B:69:THR:HG22	1.69	0.58
1:F:296:ILE:HG22	1:F:300:ASP:HB2	1.84	0.58
1:C:75:ALA:HB2	1:C:80:LEU:HD12	1.85	0.58
1:A:297:ARG:NH2	1:A:329:GLY:O	2.36	0.58
1:A:104:TYR:CG	1:B:63:GLU:O	2.57	0.58
1:A:412:ILE:HG21	1:A:438:PHE:HE2	1.69	0.58
1:F:233:GLU:CG	1:F:315:GLY:HA3	2.34	0.58
1:E:321:TYR:H	1:E:360:LEU:HB2	1.69	0.58
1:B:133:GLU:CA	1:B:134:ASP:HB2	2.32	0.57
1:B:24:VAL:O	1:B:28:PRO:HB3	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:266:GLY:HA2	1:E:267:LYS:O	2.04	0.57
1:E:412:ILE:HG21	1:E:438:PHE:HE2	1.70	0.57
1:A:30:ALA:O	1:A:33:PRO:HD2	2.03	0.57
1:C:307:ARG:NE	1:D:36:GLU:CD	2.58	0.57
1:A:378:SER:O	1:A:382:GLU:HG2	2.04	0.57
1:B:314:LEU:HD23	1:B:315:GLY:N	2.20	0.57
1:C:296:ILE:CG2	1:C:300:ASP:HB2	2.34	0.57
1:C:174:GLU:CD	1:C:178:ASN:CB	2.73	0.56
1:D:104:TYR:CB	1:D:105:TYR:HB2	2.32	0.56
1:E:28:PRO:C	1:E:30:ALA:H	2.08	0.56
1:A:412:ILE:HG21	1:A:438:PHE:CE2	2.39	0.56
1:C:104:TYR:H	1:C:107:ARG:H	1.53	0.56
1:C:269:THR:HB	1:C:272:ASP:HB2	1.86	0.56
1:B:412:ILE:HG21	1:B:438:PHE:HE2	1.69	0.56
1:A:162:ILE:HD13	1:F:288:ILE:HB	1.86	0.56
1:F:133:GLU:CA	1:F:134:ASP:HB2	2.32	0.56
1:C:103:GLU:N	1:C:104:TYR:CB	2.69	0.56
1:C:40:PRO:HG2	1:C:53:HIS:HD2	1.71	0.56
1:A:246:GLN:HE22	1:B:420:ARG:CB	2.18	0.56
1:B:233:GLU:HG2	1:B:315:GLY:HA3	1.89	0.56
1:D:51:ILE:HD11	1:D:83:ILE:HG21	1.87	0.56
1:B:296:ILE:CG2	1:B:300:ASP:HB2	2.36	0.55
1:A:306:ARG:NH2	1:B:103:GLU:CD	2.59	0.55
1:C:302:ARG:HH12	1:D:60:ASP:HA	1.70	0.55
1:B:207:ILE:CD1	1:B:386:ILE:HG22	2.36	0.55
1:C:32:VAL:HB	1:C:33:PRO:HD3	1.88	0.55
1:D:133:GLU:H	1:D:134:ASP:HB3	1.62	0.55
1:A:231:THR:HG23	1:A:233:GLU:H	1.71	0.55
1:E:412:ILE:HG21	1:E:438:PHE:CE2	2.42	0.55
1:B:296:ILE:HG22	1:B:300:ASP:HB2	1.88	0.55
1:E:296:ILE:HG22	1:E:300:ASP:HB2	1.89	0.55
1:B:268:LEU:CB	1:C:177:HIS:HE1	2.07	0.55
1:B:208:VAL:HB	1:B:360:LEU:HD23	1.87	0.55
1:F:28:PRO:C	1:F:30:ALA:H	2.09	0.55
1:B:262:ASN:OD1	1:B:268:LEU:HG	2.07	0.55
1:C:21:LEU:HB3	1:C:92:LEU:HD13	1.88	0.55
1:F:316:MET:HG2	1:F:356:PRO:HG2	1.88	0.55
1:C:174:GLU:CD	1:C:178:ASN:HB3	2.26	0.54
1:A:302:ARG:CG	1:A:349:LEU:HD13	2.37	0.54
1:B:228:ALA:HB1	1:B:286:ALA:HB1	1.89	0.54
1:A:41:GLU:OE1	1:A:41:GLU:N	2.34	0.54
1:A:175:MET:O	1:A:179:ARG:HD2	2.06	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:267:LYS:O	1:B:268:LEU:HB2	2.08	0.54
1:E:302:ARG:HG2	1:E:349:LEU:HD13	1.89	0.54
1:A:292:ASP:O	1:B:351:ARG:CD	2.56	0.54
1:C:104:TYR:HD1	1:C:105:TYR:CG	2.26	0.54
1:B:132:ARG:NH1	1:B:135:GLU:OE1	2.39	0.54
1:F:381:ARG:HH22	1:F:388:GLN:HE22	1.55	0.54
1:E:105:TYR:HE2	1:F:68:VAL:HB	1.71	0.54
1:A:294:PRO:HD3	1:B:351:ARG:HD2	1.89	0.53
1:D:104:TYR:HB3	1:D:105:TYR:CB	2.35	0.53
1:A:245:GLN:HE22	1:B:202:ARG:NH1	2.06	0.53
1:C:294:PRO:HB2	1:D:381:ARG:CG	2.38	0.53
1:D:207:ILE:CD1	1:D:390:ALA:HB2	2.38	0.53
1:E:133:GLU:CA	1:E:134:ASP:HB2	2.33	0.53
1:A:64:PRO:O	1:A:69:THR:HG21	2.08	0.53
1:D:145:ARG:CD	1:D:328:SER:OG	2.52	0.53
1:E:62:GLY:CA	1:E:63:GLU:HB3	2.39	0.53
1:C:231:THR:HG23	1:C:233:GLU:H	1.74	0.53
1:A:314:LEU:HD23	1:A:315:GLY:N	2.23	0.53
1:A:262:ASN:HD21	1:A:268:LEU:HA	1.74	0.53
1:D:381:ARG:HH22	1:D:388:GLN:HE22	1.56	0.53
1:B:30:ALA:HB1	1:B:102:VAL:HG21	1.90	0.53
1:F:62:GLY:CA	1:F:63:GLU:CB	2.87	0.53
1:E:269:THR:HB	1:E:272:ASP:HB2	1.90	0.53
1:E:267:LYS:O	1:E:268:LEU:HB2	2.09	0.53
1:F:233:GLU:HG2	1:F:315:GLY:HA3	1.90	0.53
1:E:296:ILE:CG2	1:E:300:ASP:HB2	2.39	0.53
1:C:104:TYR:HE2	1:D:63:GLU:HB2	1.75	0.52
1:B:105:TYR:O	1:B:109:VAL:HG23	2.10	0.52
1:A:302:ARG:HG2	1:A:349:LEU:HD13	1.91	0.52
1:D:71:THR:HG22	1:D:89:LEU:HD13	1.90	0.52
1:B:12:GLN:HE21	1:B:14:ILE:HG12	1.74	0.52
1:D:228:ALA:HB1	1:D:286:ALA:HB1	1.91	0.52
1:B:412:ILE:HG21	1:B:438:PHE:CE2	2.44	0.52
1:B:320:ASP:HA	1:B:360:LEU:HD12	1.90	0.52
1:C:294:PRO:HB2	1:D:381:ARG:HE	1.63	0.52
1:A:166:LEU:HD22	1:F:280:MET:HG2	1.91	0.52
1:D:61:ARG:CB	1:D:62:GLY:CA	2.87	0.52
1:E:330:ARG:CZ	1:F:149:GLU:HA	2.39	0.52
1:B:302:ARG:NH2	1:B:348:ALA:HB1	2.24	0.52
1:C:348:ALA:HB2	1:D:61:ARG:O	2.10	0.52
1:F:104:TYR:HB3	1:F:105:TYR:CB	2.35	0.52
1:F:104:TYR:CB	1:F:105:TYR:HB2	2.38	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:LYS:HB3	1:F:290:ILE:O	2.09	0.52
1:F:148:MET:O	1:F:149:GLU:HG3	2.10	0.52
1:E:207:ILE:HD13	1:E:386:ILE:CG2	2.38	0.52
1:D:141:ASP:C	1:D:328:SER:HB2	2.30	0.52
1:E:265:THR:HB	1:E:267:LYS:HD2	1.92	0.52
1:E:265:THR:CG2	1:F:423:PRO:HB3	2.33	0.52
1:A:162:ILE:HG22	1:A:163:LYS:N	2.25	0.52
1:D:211:ARG:HH11	1:D:368:GLU:HG3	1.75	0.52
1:B:392:ILE:HA	1:B:418:LYS:O	2.10	0.52
1:F:197:THR:O	1:F:198:SER:HB2	2.10	0.52
1:C:161:ASN:ND2	1:C:163:LYS:HG2	2.25	0.52
1:A:104:TYR:CD2	1:B:63:GLU:O	2.62	0.51
1:C:348:ALA:CB	1:D:61:ARG:O	2.58	0.51
1:B:104:TYR:HA	1:B:106:ALA:H	1.75	0.51
1:E:83:ILE:HG22	1:E:84:GLY:H	1.76	0.51
1:C:28:PRO:C	1:C:30:ALA:N	2.63	0.51
1:D:31:LEU:HD22	1:D:65:VAL:HG21	1.93	0.51
1:F:105:TYR:O	1:F:109:VAL:HG23	2.10	0.51
1:D:197:THR:O	1:D:198:SER:HB2	2.11	0.51
1:C:63:GLU:H	1:C:64:PRO:CA	2.21	0.51
1:B:269:THR:HB	1:B:272:ASP:HB2	1.93	0.51
1:F:12:GLN:HE21	1:F:14:ILE:HD11	1.75	0.51
1:C:174:GLU:OE1	1:C:178:ASN:ND2	2.33	0.51
1:E:61:ARG:CB	1:E:62:GLY:CA	2.87	0.51
1:A:162:ILE:O	1:A:165:ILE:N	2.44	0.51
1:E:51:ILE:HD11	1:E:83:ILE:HG21	1.92	0.51
1:B:266:GLY:HA2	1:B:267:LYS:O	2.11	0.50
1:F:71:THR:HG22	1:F:89:LEU:HD12	1.93	0.50
1:B:45:ARG:O	1:B:46:ALA:C	2.50	0.50
1:E:103:GLU:N	1:E:104:TYR:HB2	2.26	0.50
1:A:173:ILE:HG22	1:A:173:ILE:O	2.11	0.50
1:B:74:LEU:HD13	1:B:83:ILE:HD11	1.93	0.50
1:B:25:PHE:CZ	1:B:89:LEU:HD22	2.46	0.50
1:E:321:TYR:HA	1:E:360:LEU:O	2.12	0.50
1:C:74:LEU:HD22	1:C:83:ILE:HD11	1.93	0.50
1:B:135:GLU:HB3	1:B:138:VAL:HB	1.94	0.50
1:D:265:THR:O	1:D:265:THR:HG22	2.11	0.50
1:D:262:ASN:HD21	1:D:268:LEU:HA	1.75	0.50
1:A:378:SER:CB	1:F:241:GLU:HG3	2.40	0.50
1:C:50:LYS:NZ	1:C:82:GLU:OE2	2.32	0.50
1:D:32:VAL:HB	1:D:33:PRO:CD	2.36	0.50
1:B:216:LYS:HB2	1:B:360:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:412:ILE:HG21	1:D:438:PHE:HE2	1.76	0.50
1:F:66:ASP:OD1	1:F:66:ASP:C	2.48	0.50
1:B:133:GLU:N	1:B:134:ASP:CB	2.33	0.50
1:B:280:MET:SD	1:C:170:TYR:CD1	3.04	0.50
1:C:175:MET:O	1:C:179:ARG:HD3	2.12	0.50
1:A:321:TYR:CE1	1:A:324:LEU:HG	2.47	0.50
1:B:378:SER:O	1:B:382:GLU:HG2	2.12	0.50
1:A:128:ASP:HB3	1:A:139:LEU:HD21	1.92	0.50
1:A:294:PRO:HA	1:B:351:ARG:HH12	1.77	0.49
1:A:294:PRO:CA	1:B:351:ARG:NH1	2.74	0.49
1:E:290:ILE:O	1:F:160:LYS:HB3	2.12	0.49
1:A:162:ILE:HG23	1:A:166:LEU:HD12	1.94	0.49
1:D:412:ILE:HG21	1:D:438:PHE:CE2	2.47	0.49
1:C:241:GLU:HG3	1:D:378:SER:CB	2.40	0.49
1:C:66:ASP:H	1:C:69:THR:HG22	1.77	0.49
1:A:58:VAL:HG13	1:A:63:GLU:HG2	1.95	0.49
1:E:74:LEU:HD22	1:E:83:ILE:HD11	1.94	0.49
1:D:28:PRO:C	1:D:30:ALA:H	2.16	0.49
1:D:61:ARG:HB2	1:D:62:GLY:CA	2.33	0.49
1:E:104:TYR:OH	1:F:63:GLU:HB2	2.11	0.49
1:F:74:LEU:HD13	1:F:83:ILE:CD1	2.42	0.49
1:D:38:LEU:HD11	1:D:106:ALA:HA	1.93	0.49
1:F:259:ASN:O	1:F:262:ASN:HB3	2.12	0.49
1:E:198:SER:H	1:E:199:GLY:HA2	1.76	0.49
1:C:266:GLY:HA2	1:C:267:LYS:O	2.13	0.49
1:E:104:TYR:CD1	1:E:104:TYR:C	2.84	0.49
1:C:197:THR:O	1:C:198:SER:HB2	2.12	0.49
1:F:378:SER:O	1:F:382:GLU:HG2	2.13	0.49
1:D:234:ASN:HB2	1:D:313:GLY:O	2.13	0.49
1:D:231:THR:HG23	1:D:233:GLU:H	1.78	0.49
1:D:314:LEU:HD23	1:D:315:GLY:N	2.27	0.49
1:A:414:ILE:HD11	1:A:429:LEU:HD12	1.95	0.49
1:C:267:LYS:O	1:C:268:LEU:HB2	2.12	0.48
1:B:212:PRO:O	1:B:213:SER:HB2	2.13	0.48
1:A:302:ARG:O	1:A:306:ARG:HB2	2.13	0.48
1:A:161:ASN:O	1:A:162:ILE:C	2.52	0.48
1:C:51:ILE:HD11	1:C:83:ILE:HG21	1.94	0.48
1:A:134:ASP:O	1:A:135:GLU:HG3	2.13	0.48
1:F:233:GLU:HG3	1:F:315:GLY:HA3	1.96	0.48
1:C:144:ASP:O	1:C:145:ARG:C	2.51	0.48
1:F:147:ILE:O	1:F:147:ILE:CG2	2.61	0.48
1:C:71:THR:HG22	1:C:89:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:273:TRP:HZ3	1:C:177:HIS:ND1	2.11	0.48
1:B:68:VAL:HG12	1:B:69:THR:N	2.28	0.48
1:A:263:LEU:HD23	1:A:268:LEU:HD11	1.96	0.48
1:C:378:SER:O	1:C:382:GLU:HG2	2.13	0.48
1:D:135:GLU:HB3	1:D:138:VAL:HB	1.95	0.48
1:A:294:PRO:HG3	1:B:348:ALA:CB	2.44	0.48
1:B:28:PRO:C	1:B:30:ALA:H	2.16	0.48
1:F:101:ASN:HB3	1:F:105:TYR:CD1	2.48	0.48
1:E:30:ALA:O	1:E:33:PRO:HD2	2.13	0.48
1:E:316:MET:HG2	1:E:356:PRO:HG2	1.96	0.48
1:D:23:ALA:HB1	1:D:102:VAL:HG22	1.94	0.48
1:B:132:ARG:HD2	1:B:139:LEU:HG	1.95	0.48
1:E:66:ASP:H	1:E:69:THR:CG2	2.21	0.48
1:B:297:ARG:NH2	1:B:329:GLY:O	2.47	0.48
1:D:53:HIS:HE1	1:D:57:ARG:NH1	2.11	0.48
1:A:104:TYR:O	1:A:108:ILE:HG12	2.14	0.48
1:D:262:ASN:OD1	1:D:268:LEU:HG	2.14	0.48
1:C:302:ARG:NH1	1:D:59:ALA:O	2.47	0.48
1:D:263:LEU:HD23	1:D:268:LEU:HD11	1.95	0.48
1:A:160:LYS:CB	1:F:290:ILE:O	2.62	0.48
1:D:316:MET:HG2	1:D:356:PRO:HG2	1.96	0.48
1:F:184:THR:N	1:F:198:SER:O	2.47	0.47
1:D:314:LEU:HD21	1:D:317:ILE:HG13	1.96	0.47
1:E:414:ILE:HD11	1:E:429:LEU:HD12	1.96	0.47
1:E:268:LEU:HD13	1:E:273:TRP:CE3	2.50	0.47
1:D:33:PRO:HA	1:D:36:GLU:OE2	2.14	0.47
1:D:50:LYS:NZ	1:D:82:GLU:OE2	2.46	0.47
1:E:211:ARG:HH11	1:E:368:GLU:HG3	1.79	0.47
1:C:102:VAL:H	1:C:105:TYR:HD1	1.63	0.47
1:E:259:ASN:O	1:E:262:ASN:HB3	2.15	0.47
1:A:296:ILE:HG22	1:A:297:ARG:O	2.14	0.47
1:B:62:GLY:HA2	1:B:63:GLU:HA	1.59	0.47
1:D:268:LEU:HD13	1:D:273:TRP:CE3	2.49	0.47
1:D:267:LYS:O	1:D:268:LEU:HB2	2.14	0.47
1:C:161:ASN:HD22	1:C:163:LYS:HG2	1.80	0.47
1:A:12:GLN:HE21	1:A:14:ILE:HG12	1.80	0.47
1:B:263:LEU:HD23	1:B:268:LEU:HD11	1.95	0.47
1:A:86:VAL:HA	1:A:89:LEU:HD12	1.97	0.47
1:B:439:VAL:HG12	1:B:440:ASN:N	2.29	0.47
1:E:233:GLU:HG2	1:E:315:GLY:HA3	1.97	0.47
1:A:206:ILE:HA	1:A:392:ILE:HG23	1.97	0.47
1:C:174:GLU:OE2	1:C:178:ASN:CB	2.59	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:GLU:CG	1:A:315:GLY:HA3	2.44	0.47
1:C:234:ASN:HB2	1:C:313:GLY:O	2.15	0.47
1:D:216:LYS:HB2	1:D:360:LEU:HD22	1.96	0.47
1:D:198:SER:H	1:D:199:GLY:HA2	1.75	0.47
1:F:19:ALA:O	1:F:23:ALA:HB2	2.15	0.47
1:A:174:GLU:OE2	1:A:175:MET:HG2	2.15	0.47
1:B:145:ARG:HD2	1:B:330:ARG:CZ	2.45	0.47
1:C:293:THR:HA	1:C:294:PRO:HD2	1.54	0.46
1:B:102:VAL:O	1:B:105:TYR:HB2	2.15	0.46
1:E:10:PRO:HA	1:E:11:PRO:HD2	1.77	0.46
1:E:24:VAL:HG11	1:E:55:MET:SD	2.55	0.46
1:E:207:ILE:CD1	1:E:386:ILE:HG22	2.43	0.46
1:C:302:ARG:NH1	1:D:60:ASP:HA	2.30	0.46
1:C:219:PHE:CE2	1:C:223:ILE:HD11	2.50	0.46
1:C:14:ILE:CD1	1:C:45:ARG:HG3	2.45	0.46
1:D:61:ARG:HD3	1:D:63:GLU:OE2	2.16	0.46
1:F:207:ILE:HD12	1:F:390:ALA:CB	2.34	0.46
1:A:198:SER:N	1:A:199:GLY:CA	2.75	0.46
1:D:208:VAL:HB	1:D:360:LEU:HD23	1.98	0.46
1:E:245:GLN:NE2	1:F:168:GLN:OE1	2.48	0.46
1:A:416:ILE:O	1:A:424:VAL:HG13	2.15	0.46
1:E:197:THR:O	1:E:198:SER:HB2	2.15	0.46
1:F:32:VAL:HB	1:F:33:PRO:CD	2.39	0.46
1:D:64:PRO:HB2	1:D:65:VAL:H	1.59	0.46
1:A:63:GLU:N	1:A:64:PRO:HA	2.28	0.46
1:D:74:LEU:HD22	1:D:83:ILE:HD11	1.98	0.46
1:E:216:LYS:HB2	1:E:360:LEU:HD22	1.97	0.45
1:F:74:LEU:HD13	1:F:83:ILE:HD11	1.98	0.45
1:F:207:ILE:CD1	1:F:390:ALA:HB2	2.33	0.45
1:E:233:GLU:CG	1:E:315:GLY:HA3	2.46	0.45
1:C:174:GLU:CD	1:C:178:ASN:HB2	2.37	0.45
1:E:101:ASN:HB2	1:E:105:TYR:CE1	2.51	0.45
1:D:47:ALA:HB1	1:D:83:ILE:HG23	1.97	0.45
1:A:168:GLN:O	1:A:170:TYR:N	2.49	0.45
1:F:76:ALA:C	1:F:78:GLU:H	2.20	0.45
1:C:184:THR:N	1:C:198:SER:O	2.50	0.45
1:D:273:TRP:CH2	1:E:173:ILE:CG2	2.98	0.45
1:E:302:ARG:O	1:E:306:ARG:HB2	2.16	0.45
1:F:135:GLU:HB3	1:F:138:VAL:HB	1.97	0.45
1:B:11:PRO:HG2	1:B:116:ARG:HG2	1.97	0.45
1:B:263:LEU:HD22	1:C:173:ILE:HG23	1.99	0.45
1:A:25:PHE:HZ	1:A:89:LEU:HD22	1.82	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:LEU:HB2	1:A:177:HIS:HD2	1.81	0.45
1:B:102:VAL:O	1:B:105:TYR:CB	2.64	0.45
1:D:32:VAL:CB	1:D:33:PRO:HD3	2.41	0.45
1:B:202:ARG:HA	1:B:356:PRO:HD3	1.99	0.45
1:F:24:VAL:HG11	1:F:55:MET:SD	2.57	0.45
1:C:268:LEU:HD13	1:C:273:TRP:CE3	2.51	0.45
1:E:208:VAL:HB	1:E:360:LEU:HD23	1.98	0.45
1:D:321:TYR:CZ	1:D:324:LEU:HG	2.52	0.45
1:A:53:HIS:HE1	1:A:57:ARG:HH11	1.62	0.45
1:A:169:THR:O	1:A:169:THR:HG22	2.17	0.45
1:E:268:LEU:HD13	1:E:273:TRP:CZ3	2.52	0.45
1:C:86:VAL:HA	1:C:89:LEU:HD12	1.99	0.45
1:D:53:HIS:CE1	1:D:57:ARG:HH11	2.35	0.45
1:E:163:LYS:HG3	1:E:164:ASP:N	2.32	0.45
1:B:363:LEU:HD23	1:B:380:ILE:HG23	1.99	0.45
1:B:105:TYR:HA	1:B:105:TYR:HD2	1.71	0.45
1:E:262:ASN:HD21	1:E:268:LEU:HA	1.82	0.45
1:B:386:ILE:HG13	1:B:386:ILE:H	1.44	0.45
1:F:132:ARG:NH1	1:F:135:GLU:OE1	2.50	0.45
1:E:234:ASN:HB2	1:E:313:GLY:O	2.16	0.45
1:B:347:LYS:HE3	1:B:351:ARG:NH2	2.32	0.44
1:C:97:PRO:HD2	1:C:98:THR:HG22	1.99	0.44
1:C:71:THR:HG22	1:C:89:LEU:CD1	2.47	0.44
1:C:302:ARG:O	1:C:306:ARG:HB2	2.17	0.44
1:F:24:VAL:HA	1:F:30:ALA:HB3	2.00	0.44
1:B:269:THR:CB	1:B:272:ASP:HB2	2.47	0.44
1:D:416:ILE:O	1:D:424:VAL:HG13	2.16	0.44
1:C:110:GLU:O	1:C:114:VAL:HG23	2.16	0.44
1:C:206:ILE:HA	1:C:392:ILE:HG23	1.98	0.44
1:C:30:ALA:HB1	1:C:102:VAL:HG21	1.99	0.44
1:E:99:ALA:O	1:E:102:VAL:HG23	2.17	0.44
1:A:381:ARG:HH22	1:A:388:GLN:NE2	2.09	0.44
1:A:192:GLU:HB3	1:A:427:VAL:CG1	2.48	0.44
1:D:302:ARG:O	1:D:306:ARG:HB2	2.17	0.44
1:E:314:LEU:HD23	1:E:315:GLY:N	2.32	0.44
1:B:414:ILE:HD11	1:B:429:LEU:HD12	2.00	0.44
1:A:15:GLU:OE2	1:B:86:VAL:HG11	2.17	0.44
1:C:294:PRO:HB2	1:D:381:ARG:HG2	2.00	0.44
1:A:11:PRO:HG3	1:A:119:ILE:CD1	2.47	0.44
1:B:262:ASN:HD21	1:B:268:LEU:HA	1.82	0.44
1:A:159:PHE:HD1	1:A:160:LYS:N	2.13	0.44
1:A:28:PRO:C	1:A:30:ALA:H	2.20	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:200:PHE:HE2	1:A:223:ILE:HD13	1.82	0.44
1:A:411:ILE:HD11	1:A:441:LEU:HD21	1.99	0.44
1:C:212:PRO:O	1:C:213:SER:HB2	2.17	0.44
1:C:307:ARG:NE	1:D:36:GLU:OE2	2.50	0.44
1:C:321:TYR:H	1:C:360:LEU:HB2	1.83	0.44
1:D:141:ASP:C	1:D:143:ALA:N	2.69	0.44
1:A:246:GLN:NE2	1:B:420:ARG:CB	2.70	0.44
1:F:268:LEU:HD13	1:F:273:TRP:CE3	2.52	0.44
1:B:145:ARG:HD2	1:B:330:ARG:NH2	2.33	0.43
1:D:138:VAL:HG22	1:D:297:ARG:NH1	2.33	0.43
1:C:63:GLU:N	1:C:64:PRO:CA	2.81	0.43
1:F:262:ASN:O	1:F:266:GLY:HA2	2.18	0.43
1:F:267:LYS:O	1:F:268:LEU:CB	2.65	0.43
1:C:40:PRO:HG2	1:C:53:HIS:CD2	2.52	0.43
1:E:314:LEU:HD21	1:E:317:ILE:HG13	2.00	0.43
1:D:210:ALA:HB3	1:D:216:LYS:HB3	1.99	0.43
1:B:32:VAL:HB	1:B:33:PRO:HD3	2.00	0.43
1:E:132:ARG:HD2	1:E:139:LEU:HG	2.00	0.43
1:F:223:ILE:HG22	1:F:316:MET:HE1	2.01	0.43
1:B:11:PRO:HG2	1:B:116:ARG:CG	2.47	0.43
1:B:231:THR:HG23	1:B:233:GLU:H	1.83	0.43
1:D:321:TYR:CE1	1:D:324:LEU:HG	2.53	0.43
1:D:212:PRO:O	1:D:213:SER:HB2	2.18	0.43
1:F:53:HIS:HE1	1:F:57:ARG:NH1	2.17	0.43
1:B:268:LEU:HD13	1:B:273:TRP:CE3	2.53	0.43
1:B:268:LEU:CD1	1:C:177:HIS:CE1	2.98	0.43
1:B:347:LYS:HG3	1:B:351:ARG:NH1	2.33	0.43
1:E:19:ALA:O	1:E:23:ALA:CB	2.65	0.43
1:C:74:LEU:HD13	1:C:83:ILE:HD11	2.01	0.43
1:B:188:THR:HG23	1:B:223:ILE:HG23	2.00	0.43
1:D:280:MET:HG2	1:E:166:LEU:HD22	2.01	0.43
1:B:99:ALA:O	1:B:102:VAL:HG23	2.19	0.43
1:A:55:MET:HG3	1:A:65:VAL:HG11	2.01	0.43
1:A:268:LEU:HD13	1:A:273:TRP:CZ3	2.54	0.43
1:F:293:THR:HA	1:F:294:PRO:HD2	1.81	0.43
1:F:208:VAL:HB	1:F:360:LEU:HD23	2.01	0.43
1:A:302:ARG:HG3	1:A:349:LEU:HD13	2.01	0.43
1:B:61:ARG:CB	1:B:62:GLY:CA	2.93	0.43
1:D:14:ILE:HD13	1:D:14:ILE:HA	1.90	0.43
1:C:210:ALA:HB3	1:C:216:LYS:HB3	2.00	0.43
1:E:104:TYR:OH	1:F:63:GLU:CG	2.67	0.43
1:C:321:TYR:CE1	1:C:324:LEU:HG	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:233:GLU:HG2	1:C:315:GLY:HA3	2.00	0.43
1:A:259:ASN:O	1:A:262:ASN:HB3	2.19	0.43
1:F:74:LEU:HD22	1:F:83:ILE:HD11	2.01	0.43
1:B:188:THR:HG21	1:B:193:LEU:HD23	2.00	0.43
1:E:253:CYS:SG	1:E:263:LEU:HD12	2.59	0.43
1:F:439:VAL:HG12	1:F:440:ASN:N	2.34	0.43
1:C:61:ARG:CB	1:C:62:GLY:CA	2.84	0.43
1:D:39:ILE:O	1:D:41:GLU:N	2.52	0.43
1:A:179:ARG:O	1:A:180:ASP:C	2.57	0.43
1:F:308:LEU:HD23	1:F:314:LEU:HD12	1.99	0.43
1:E:293:THR:HB	1:E:296:ILE:HG12	2.00	0.42
1:D:148:MET:O	1:D:149:GLU:HG3	2.19	0.42
1:E:148:MET:O	1:E:149:GLU:HG3	2.18	0.42
1:D:209:ALA:HA	1:D:361:SER:O	2.19	0.42
1:C:62:GLY:HA2	1:C:63:GLU:HA	1.83	0.42
1:B:321:TYR:CZ	1:B:324:LEU:HG	2.55	0.42
1:B:273:TRP:HZ3	1:C:177:HIS:CE1	2.37	0.42
1:D:66:ASP:N	1:D:69:THR:HG22	2.28	0.42
1:D:69:THR:HG23	1:D:70:VAL:N	2.34	0.42
1:E:71:THR:HA	1:E:74:LEU:HD12	2.02	0.42
1:F:266:GLY:HA2	1:F:267:LYS:O	2.20	0.42
1:B:240:LEU:HD22	1:B:293:THR:O	2.18	0.42
1:F:53:HIS:CE1	1:F:57:ARG:HH11	2.37	0.42
1:B:96:VAL:HA	1:B:97:PRO:HD3	1.91	0.42
1:D:135:GLU:HG2	1:D:330:ARG:NE	2.35	0.42
1:D:378:SER:O	1:D:382:GLU:HG2	2.19	0.42
1:C:265:THR:HB	1:C:267:LYS:HD2	2.02	0.42
1:C:103:GLU:H	1:C:104:TYR:HB2	1.84	0.42
1:F:32:VAL:CB	1:F:33:PRO:HD3	2.39	0.42
1:A:161:ASN:O	1:A:163:LYS:N	2.52	0.42
1:A:185:GLY:HA3	1:A:201:GLN:HG2	2.02	0.42
1:A:210:ALA:HB2	1:A:396:LEU:HB2	2.01	0.42
1:C:96:VAL:HA	1:C:97:PRO:HD3	1.83	0.42
1:C:314:LEU:HD21	1:C:317:ILE:HG13	2.02	0.42
1:E:161:ASN:OD1	1:E:162:ILE:N	2.53	0.42
1:B:76:ALA:HA	1:F:133:GLU:HB3	2.00	0.42
1:D:24:VAL:HG13	1:D:31:LEU:HB2	2.01	0.42
1:C:14:ILE:HD11	1:C:45:ARG:HG3	2.02	0.42
1:D:53:HIS:HE1	1:D:57:ARG:HH11	1.68	0.42
1:F:198:SER:H	1:F:199:GLY:HA2	1.80	0.42
1:A:132:ARG:HD3	1:A:135:GLU:OE1	2.20	0.42
1:C:179:ARG:NE	1:C:179:ARG:HA	2.35	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:302:ARG:O	1:B:306:ARG:HB2	2.20	0.42
1:C:61:ARG:HD3	1:C:63:GLU:CD	2.40	0.42
1:B:65:VAL:HA	1:B:69:THR:HG21	2.02	0.42
1:F:28:PRO:C	1:F:30:ALA:N	2.72	0.42
1:C:74:LEU:HD13	1:C:83:ILE:CD1	2.50	0.42
1:D:388:GLN:HE21	1:D:388:GLN:HB2	1.57	0.42
1:E:267:LYS:O	1:E:268:LEU:CB	2.68	0.42
1:C:13:SER:O	1:C:14:ILE:C	2.59	0.42
1:E:378:SER:O	1:E:382:GLU:HG2	2.20	0.42
1:B:64:PRO:O	1:B:69:THR:HG21	2.20	0.41
1:A:259:ASN:HB3	1:A:262:ASN:HB3	2.01	0.41
1:A:347:LYS:HE3	1:A:351:ARG:CZ	2.50	0.41
1:B:263:LEU:CD2	1:B:268:LEU:HD11	2.50	0.41
1:F:207:ILE:CD1	1:F:386:ILE:HG22	2.46	0.41
1:A:188:THR:OG1	1:A:194:ASP:OD1	2.32	0.41
1:C:267:LYS:O	1:C:268:LEU:CB	2.67	0.41
1:B:10:PRO:HA	1:B:11:PRO:HD2	1.86	0.41
1:E:192:GLU:HB3	1:E:427:VAL:HG13	2.02	0.41
1:B:132:ARG:O	1:B:133:GLU:CB	2.68	0.41
1:C:294:PRO:CB	1:D:381:ARG:CZ	2.99	0.41
1:D:297:ARG:NH2	1:D:329:GLY:O	2.53	0.41
1:E:28:PRO:C	1:E:30:ALA:N	2.72	0.41
1:E:210:ALA:HB3	1:E:216:LYS:HB3	2.03	0.41
1:A:216:LYS:HB2	1:A:360:LEU:HD22	2.02	0.41
1:B:241:GLU:HG3	1:C:378:SER:HB3	2.02	0.41
1:D:141:ASP:OD2	1:D:297:ARG:HB2	2.21	0.41
1:E:262:ASN:OD1	1:E:268:LEU:HG	2.20	0.41
1:D:142:GLU:CA	1:D:328:SER:HB2	2.50	0.41
1:F:25:PHE:CE1	1:F:67:LEU:HD23	2.56	0.41
1:C:233:GLU:CG	1:C:315:GLY:HA3	2.51	0.41
1:F:197:THR:HA	1:F:419:GLN:OE1	2.21	0.41
1:D:267:LYS:O	1:D:268:LEU:CB	2.68	0.41
1:D:136:ILE:C	1:D:138:VAL:H	2.24	0.41
1:E:198:SER:N	1:E:199:GLY:CA	2.77	0.41
1:F:253:CYS:SG	1:F:263:LEU:HD12	2.60	0.41
1:F:96:VAL:HG22	1:F:97:PRO:HD2	2.03	0.41
1:E:133:GLU:N	1:E:134:ASP:CB	2.32	0.41
1:A:104:TYR:CD1	1:B:63:GLU:O	2.73	0.41
1:E:293:THR:HA	1:E:294:PRO:HD2	1.79	0.41
1:D:130:TYR:CE1	1:E:119:ILE:HD13	2.56	0.41
1:B:267:LYS:O	1:B:268:LEU:CB	2.68	0.41
1:A:233:GLU:HG3	1:A:315:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:GLU:HG2	1:A:315:GLY:HA3	2.03	0.41
1:E:197:THR:HA	1:E:419:GLN:OE1	2.21	0.41
1:A:321:TYR:H	1:A:360:LEU:HB2	1.86	0.41
1:F:53:HIS:HE1	1:F:57:ARG:HH11	1.68	0.41
1:C:416:ILE:O	1:C:424:VAL:HG13	2.21	0.41
1:A:74:LEU:HD22	1:A:83:ILE:HD11	2.03	0.41
1:F:414:ILE:HD11	1:F:429:LEU:HD12	2.02	0.41
1:C:209:ALA:HA	1:C:361:SER:O	2.21	0.41
1:F:148:MET:CE	1:F:148:MET:HA	2.50	0.41
1:E:104:TYR:HA	1:E:106:ALA:H	1.86	0.41
1:A:207:ILE:HD12	1:A:390:ALA:CB	2.37	0.41
1:A:262:ASN:O	1:A:266:GLY:HA2	2.21	0.41
1:A:208:VAL:HB	1:A:360:LEU:HD23	2.03	0.41
1:F:83:ILE:HB	1:F:84:GLY:H	1.62	0.41
1:E:46:ALA:O	1:E:50:LYS:HD3	2.21	0.41
1:F:222:ASN:HD22	1:F:222:ASN:N	2.18	0.41
1:D:65:VAL:HA	1:D:69:THR:HG21	2.03	0.40
1:B:102:VAL:O	1:B:106:ALA:N	2.51	0.40
1:B:47:ALA:HB1	1:B:83:ILE:HG23	2.03	0.40
1:A:74:LEU:HD13	1:A:83:ILE:CD1	2.51	0.40
1:F:192:GLU:HB3	1:F:427:VAL:HG13	2.04	0.40
1:A:42:ASP:HA	1:A:113:SER:OG	2.21	0.40
1:B:48:HIS:CD2	1:B:48:HIS:H	2.39	0.40
1:B:67:LEU:O	1:B:71:THR:CG2	2.66	0.40
1:F:231:THR:HG23	1:F:233:GLU:H	1.86	0.40
1:A:53:HIS:HE1	1:A:57:ARG:NH1	2.19	0.40
1:A:83:ILE:HB	1:A:84:GLY:H	1.73	0.40
1:A:217:THR:O	1:A:221:LEU:HG	2.20	0.40
1:A:135:GLU:HB3	1:A:138:VAL:HB	2.04	0.40
1:D:145:ARG:HH12	1:D:329:GLY:H	1.69	0.40
1:B:207:ILE:HD13	1:B:386:ILE:CG2	2.46	0.40
1:D:211:ARG:NH1	1:D:368:GLU:HG3	2.36	0.40
1:E:38:LEU:HD21	1:E:109:VAL:HB	2.03	0.40
1:A:24:VAL:HG11	1:A:55:MET:SD	2.62	0.40
1:D:71:THR:HG22	1:D:89:LEU:CD1	2.52	0.40
1:B:240:LEU:HD21	1:B:296:ILE:HG13	2.04	0.40
1:A:261:GLN:HA	1:A:264:ARG:HD2	2.04	0.40
1:C:294:PRO:CB	1:D:381:ARG:HG2	2.52	0.40
1:E:320:ASP:HA	1:E:360:LEU:HD12	2.03	0.40
1:A:168:GLN:C	1:A:170:TYR:N	2.75	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:178:ASN:ND2	1:F:97:PRO:CB[1.565]	2.12	0.08
1:C:178:ASN:CG	1:F:97:PRO:CB[1.565]	2.13	0.07

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/454 (87%)	334 (85%)	43 (11%)	18 (5%)	4	46
1	B	366/454 (81%)	308 (84%)	46 (13%)	12 (3%)	6	57
1	C	389/454 (86%)	327 (84%)	37 (10%)	25 (6%)	2	36
1	D	366/454 (81%)	308 (84%)	42 (12%)	16 (4%)	4	48
1	E	380/454 (84%)	325 (86%)	38 (10%)	17 (4%)	4	47
1	F	380/454 (84%)	331 (87%)	33 (9%)	16 (4%)	4	49
All	All	2276/2724 (84%)	1933 (85%)	239 (10%)	104 (5%)	4	46

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	134	ASP
1	A	162	ILE
1	A	179	ARG
1	A	180	ASP
1	A	266	GLY
1	A	268	LEU
1	A	321	TYR
1	B	83	ILE
1	B	104	TYR
1	B	133	GLU
1	B	268	LEU
1	B	321	TYR
1	C	63	GLU
1	C	104	TYR
1	C	133	GLU

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Mol	Chain	Res	Type
1	C	134	ASP
1	C	179	ARG
1	C	180	ASP
1	C	266	GLY
1	C	268	LEU
1	C	321	TYR
1	D	63	GLU
1	D	64	PRO
1	D	83	ILE
1	D	102	VAL
1	D	104	TYR
1	D	134	ASP
1	D	268	LEU
1	D	321	TYR
1	E	63	GLU
1	E	83	ILE
1	E	102	VAL
1	E	134	ASP
1	E	266	GLY
1	E	268	LEU
1	E	321	TYR
1	F	63	GLU
1	F	64	PRO
1	F	102	VAL
1	F	104	TYR
1	F	134	ASP
1	F	266	GLY
1	F	268	LEU
1	F	321	TYR
1	A	163	LYS
1	A	169	THR
1	A	198	SER
1	B	63	GLU
1	B	134	ASP
1	B	136	ILE
1	B	266	GLY
1	C	44	TYR
1	C	101	ASN
1	C	145	ARG
1	C	175	MET
1	D	133	GLU
1	D	136	ILE

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Mol	Chain	Res	Type
1	D	198	SER
1	D	266	GLY
1	A	133	GLU
1	A	267	LYS
1	C	116	ARG
1	C	440	ASN
1	D	78	GLU
1	E	11	PRO
1	E	133	GLU
1	E	198	SER
1	F	78	GLU
1	F	97	PRO
1	F	198	SER
1	A	64	PRO
1	B	64	PRO
1	B	101	ASN
1	B	267	LYS
1	C	64	PRO
1	C	78	GLU
1	C	95	ALA
1	C	181	GLY
1	D	40	PRO
1	D	267	LYS
1	E	49	GLN
1	E	97	PRO
1	E	104	TYR
1	E	267	LYS
1	A	365	ARG
1	C	27	ASP
1	C	83	ILE
1	C	105	TYR
1	C	267	LYS
1	E	29	ALA
1	E	101	ASN
1	F	133	GLU
1	F	267	LYS
1	A	83	ILE
1	A	136	ILE
1	D	142	GLU
1	E	64	PRO
1	A	181	GLY
1	C	102	VAL

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Mol	Chain	Res	Type
1	C	136	ILE
1	F	40	PRO
1	F	83	ILE
1	F	136	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/386 (88%)	314 (92%)	27 (8%)	18	65
1	B	314/386 (81%)	294 (94%)	20 (6%)	25	74
1	C	336/386 (87%)	318 (95%)	18 (5%)	31	79
1	D	314/386 (81%)	291 (93%)	23 (7%)	20	69
1	E	330/386 (86%)	310 (94%)	20 (6%)	26	75
1	F	330/386 (86%)	307 (93%)	23 (7%)	21	70
All	All	1965/2316 (85%)	1834 (93%)	131 (7%)	23	72

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	60	ASP
1	A	67	LEU
1	A	80	LEU
1	A	81	GLU
1	A	96	VAL
1	A	115	LEU
1	A	120	ARG
1	A	136	ILE
1	A	159	PHE
1	A	161	ASN
1	A	163	LYS
1	A	164	ASP
1	A	268	LEU
1	A	271	GLU

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Mol	Chain	Res	Type
1	A	272	ASP
1	A	278	MET
1	A	297	ARG
1	A	316	MET
1	A	321	TYR
1	A	323	GLN
1	A	339	VAL
1	A	340	SER
1	A	386	ILE
1	A	388	GLN
1	A	391	ASP
1	A	412	ILE
1	B	12	GLN
1	B	55	MET
1	B	56	LEU
1	B	80	LEU
1	B	104	TYR
1	B	128	ASP
1	B	135	GLU
1	B	136	ILE
1	B	144	ASP
1	B	147	ILE
1	B	148	MET
1	B	195	ARG
1	B	233	GLU
1	B	269	THR
1	B	271	GLU
1	B	306	ARG
1	B	321	TYR
1	B	386	ILE
1	B	388	GLN
1	B	412	ILE
1	C	26	LEU
1	C	50	LYS
1	C	61	ARG
1	C	81	GLU
1	C	115	LEU
1	C	139	LEU
1	C	141	ASP
1	C	148	MET
1	C	163	LYS
1	C	174	GLU

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Mol	Chain	Res	Type
1	C	195	ARG
1	C	271	GLU
1	C	316	MET
1	C	321	TYR
1	C	386	ILE
1	C	388	GLN
1	C	391	ASP
1	C	412	ILE
1	D	12	GLN
1	D	50	LYS
1	D	56	LEU
1	D	80	LEU
1	D	86	VAL
1	D	103	GLU
1	D	104	TYR
1	D	128	ASP
1	D	134	ASP
1	D	136	ILE
1	D	139	LEU
1	D	140	LEU
1	D	141	ASP
1	D	147	ILE
1	D	195	ARG
1	D	231	THR
1	D	268	LEU
1	D	316	MET
1	D	321	TYR
1	D	386	ILE
1	D	388	GLN
1	D	391	ASP
1	D	412	ILE
1	E	12	GLN
1	E	26	LEU
1	E	60	ASP
1	E	81	GLU
1	E	105	TYR
1	E	114	VAL
1	E	115	LEU
1	E	139	LEU
1	E	148	MET
1	E	163	LYS
1	E	171	ASP

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Mol	Chain	Res	Type
1	E	174	GLU
1	E	195	ARG
1	E	268	LEU
1	E	271	GLU
1	E	316	MET
1	E	321	TYR
1	E	386	ILE
1	E	388	GLN
1	E	412	ILE
1	F	12	GLN
1	F	50	LYS
1	F	77	SER
1	F	80	LEU
1	F	86	VAL
1	F	90	SER
1	F	103	GLU
1	F	104	TYR
1	F	128	ASP
1	F	139	LEU
1	F	148	MET
1	F	163	LYS
1	F	174	GLU
1	F	195	ARG
1	F	268	LEU
1	F	271	GLU
1	F	272	ASP
1	F	316	MET
1	F	321	TYR
1	F	345	SER
1	F	386	ILE
1	F	391	ASP
1	F	412	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	53	HIS
1	A	79	GLN
1	A	152	GLN
1	A	177	HIS
1	A	225	GLN

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Mol	Chain	Res	Type
1	A	226	ASN
1	A	245	GLN
1	A	246	GLN
1	A	323	GLN
1	A	388	GLN
1	A	436	ASN
1	B	12	GLN
1	B	53	HIS
1	B	79	GLN
1	B	225	GLN
1	B	226	ASN
1	B	323	GLN
1	B	388	GLN
1	C	12	GLN
1	C	53	HIS
1	C	172	ASN
1	C	177	HIS
1	C	225	GLN
1	C	323	GLN
1	C	388	GLN
1	D	49	GLN
1	D	53	HIS
1	D	79	GLN
1	D	225	GLN
1	D	226	ASN
1	D	323	GLN
1	D	388	GLN
1	E	53	HIS
1	E	79	GLN
1	E	225	GLN
1	E	226	ASN
1	E	245	GLN
1	E	323	GLN
1	E	388	GLN
1	F	12	GLN
1	F	53	HIS
1	F	225	GLN
1	F	323	GLN
1	F	388	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	405/454 (89%)	-0.01	4 (0%) 79 57	153, 178, 179, 207	0
1	B	376/454 (82%)	-0.01	4 (1%) 77 54	175, 178, 179, 187	0
1	C	399/454 (87%)	0.10	4 (1%) 79 57	145, 178, 179, 209	0
1	D	376/454 (82%)	0.05	9 (2%) 56 35	165, 178, 179, 184	0
1	E	392/454 (86%)	0.36	28 (7%) 16 11	169, 178, 179, 198	0
1	F	392/454 (86%)	0.06	9 (2%) 57 36	176, 178, 180, 189	0
All	All	2340/2724 (85%)	0.09	58 (2%) 54 34	145, 178, 179, 209	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	409	LYS	8.0
1	F	330	ARG	7.6
1	E	374	ARG	6.7
1	A	330	ARG	5.7
1	E	397	TYR	5.4
1	F	382	GLU	5.3
1	B	330	ARG	5.0
1	E	441	LEU	4.7
1	C	330	ARG	4.5
1	B	382	GLU	4.5
1	E	420	ARG	4.1
1	F	160	LYS	3.9
1	E	182	GLU	3.8
1	A	265	THR	3.5
1	E	310	GLN	3.4
1	E	183	ILE	3.4
1	E	329	GLY	3.4
1	B	409	LYS	3.3
1	D	330	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	368	GLU	3.3
1	E	330	ARG	3.1
1	D	264	ARG	3.1
1	E	256	GLY	3.1
1	E	184	THR	3.0
1	D	328	SER	2.9
1	A	329	GLY	2.9
1	D	381	ARG	2.9
1	C	97	PRO	2.8
1	E	260	ALA	2.8
1	D	329	GLY	2.8
1	E	307	ARG	2.7
1	C	327	GLY	2.7
1	E	384	GLY	2.7
1	F	384	GLY	2.7
1	F	184	THR	2.6
1	E	261	GLN	2.6
1	D	265	THR	2.5
1	E	421	ASN	2.5
1	F	329	GLY	2.4
1	F	409	LYS	2.4
1	E	311	GLU	2.4
1	E	259	ASN	2.3
1	F	397	TYR	2.3
1	E	383	SER	2.3
1	E	367	VAL	2.3
1	E	264	ARG	2.2
1	E	428	GLN	2.2
1	E	255	GLU	2.2
1	E	97	PRO	2.1
1	D	382	GLU	2.1
1	E	354	GLU	2.1
1	E	289	TYR	2.1
1	F	366	SER	2.1
1	D	100	ALA	2.1
1	B	368	GLU	2.0
1	A	153	ARG	2.0
1	C	179	ARG	2.0
1	D	250	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.