



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:37 AM GMT

PDB ID : 3BGW  
Title : The Structure Of A DnaB-Like Replicative Helicase And Its Interactions With Primase  
Authors : Wang, G.; Klein, M.G.; Tokonzaba, E.; Zhang, Y.; Holden, L.G.; Chen, X.S.  
Deposited on : 2007-11-27  
Resolution : 3.91 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

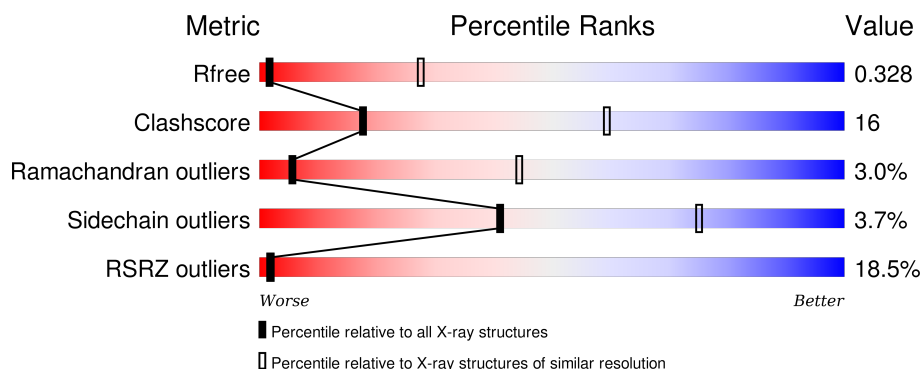
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.91 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1047 (4.32-3.52)
Clashscore	102246	1008 (4.26-3.58)
Ramachandran outliers	100387	1044 (4.30-3.54)
Sidechain outliers	100360	1035 (4.30-3.54)
RSRZ outliers	91569	1002 (4.30-3.54)

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. 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	444	<div> <div>7%</div> <div>63%</div> <div>27%</div> <div>6%</div> </div>
1	B	444	<div> <div>8%</div> <div>67%</div> <div>23%</div> <div>6%</div> </div>
1	C	444	<div> <div>27%</div> <div>67%</div> <div>24%</div> <div>6%</div> </div>
1	D	444	<div> <div>21%</div> <div>68%</div> <div>21%</div> <div>8%</div> </div>
1	E	444	<div> <div>25%</div> <div>68%</div> <div>22%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	444	<div><div></div><div>15%</div><div>65%</div><div>25%</div><div>• • 6%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19724 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 DNAB-Like Replicative Helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3298	2062	571	653	12			
1	B	419	Total	C	N	O	S	0	0	0
			3298	2062	571	653	12			
1	C	419	Total	C	N	O	S	0	0	0
			3298	2062	571	653	12			
1	D	409	Total	C	N	O	S	0	0	0
			3234	2029	561	632	12			
1	E	419	Total	C	N	O	S	0	0	0
			3298	2062	571	653	12			
1	F	419	Total	C	N	O	S	0	0	0
			3298	2062	571	653	12			

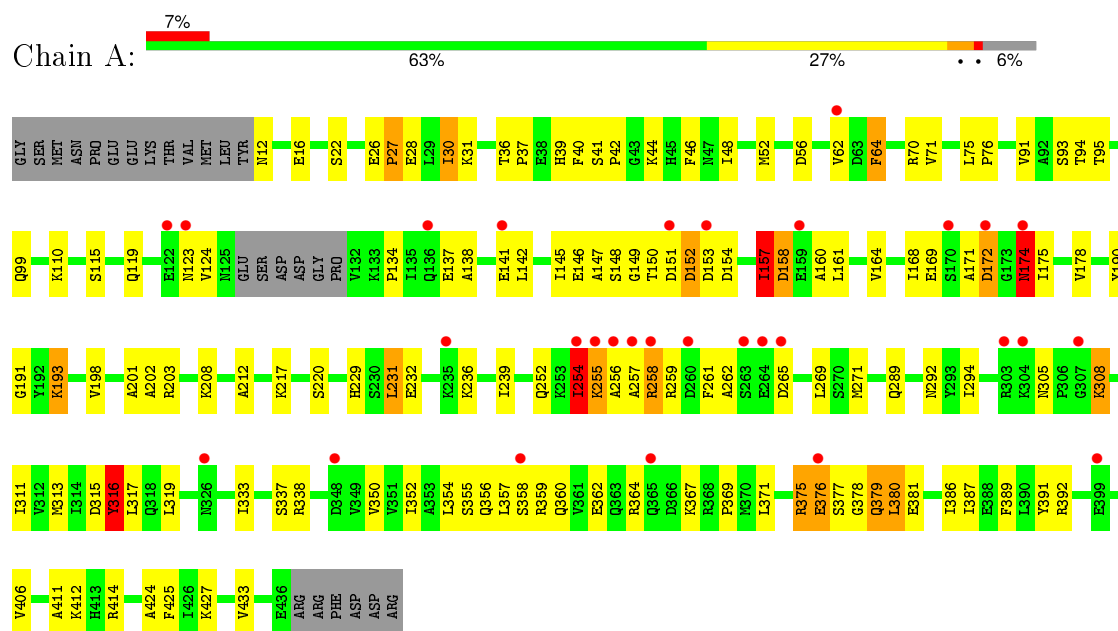
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q38152
A	0	SER	-	EXPRESSION TAG	UNP Q38152
B	-1	GLY	-	EXPRESSION TAG	UNP Q38152
B	0	SER	-	EXPRESSION TAG	UNP Q38152
C	-1	GLY	-	EXPRESSION TAG	UNP Q38152
C	0	SER	-	EXPRESSION TAG	UNP Q38152
D	-1	GLY	-	EXPRESSION TAG	UNP Q38152
D	0	SER	-	EXPRESSION TAG	UNP Q38152
E	-1	GLY	-	EXPRESSION TAG	UNP Q38152
E	0	SER	-	EXPRESSION TAG	UNP Q38152
F	-1	GLY	-	EXPRESSION TAG	UNP Q38152
F	0	SER	-	EXPRESSION TAG	UNP Q38152

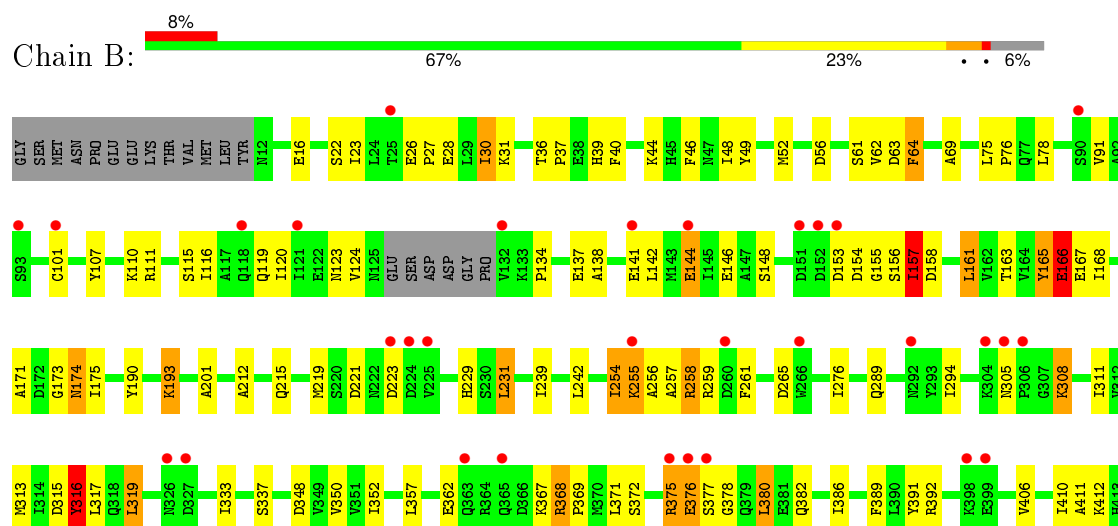
### 3 Residue-property plots

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.

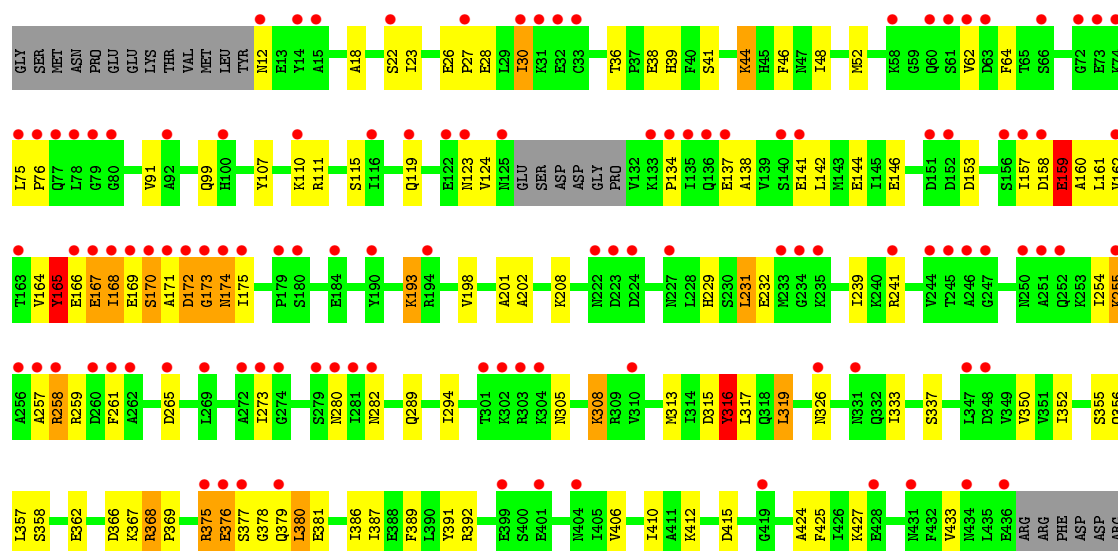
#### • Molecule 1: DNAB-Like Replicative Helicase



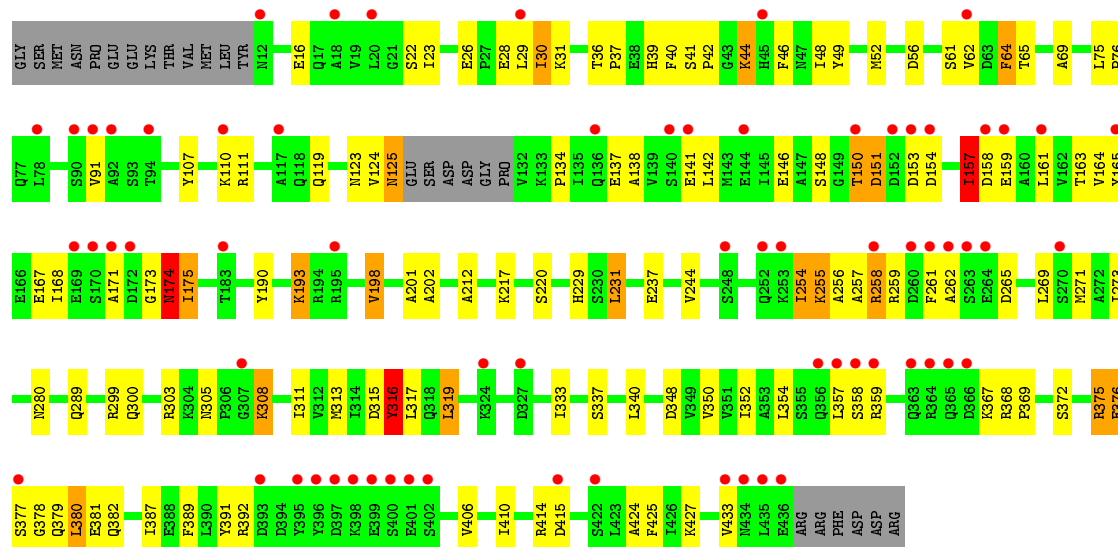
#### • Molecule 1: DNAB-Like Replicative Helicase







• Molecule 1: DNAB-Like Replicative Helicase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.63Å 184.41Å 184.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 3.91 38.80 – 3.91	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.81-3.91) 97.4 (38.80-3.91)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.68 (at 3.87Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.338 , 0.349 0.321 , 0.328	Depositor DCC
$R_{free}$ test set	1750 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 140.0	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 35080 reflections	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	19724	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.32	1/3345 (0.0%)	0.41	0/4507
1	B	0.26	0/3345	0.40	0/4507
1	C	0.30	2/3345 (0.1%)	0.39	0/4507
1	D	0.27	0/3280	0.39	0/4417
1	E	0.32	2/3345 (0.1%)	0.41	0/4507
1	F	0.34	4/3345 (0.1%)	0.42	1/4507 (0.0%)
All	All	0.30	9/20005 (0.0%)	0.40	1/26952 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	173	GLY	C-O	-8.20	1.10	1.23
1	F	174	ASN	CB-CG	-7.97	1.32	1.51
1	E	159	GLU	CD-OE2	6.62	1.32	1.25
1	A	174	ASN	CB-CG	-6.20	1.36	1.51
1	C	174	ASN	CB-CG	-6.08	1.37	1.51
1	C	174	ASN	CG-OD1	-5.54	1.11	1.24
1	F	174	ASN	C-O	-5.23	1.13	1.23
1	F	174	ASN	CA-C	-5.16	1.39	1.52
1	F	174	ASN	CA-CB	-5.13	1.39	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	174	ASN	N-CA-C	6.07	127.39	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	3298	0	3279	138	0
1	B	3298	0	3279	119	0
1	C	3298	0	3279	121	0
1	D	3234	0	3234	107	0
1	E	3298	0	3279	114	0
1	F	3298	0	3277	127	0
All	All	19724	0	19627	626	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 16.

All (626) 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:D:52:MET:HG3	1:D:62:VAL:HG11	1.28	1.08
1:E:232:GLU:OE2	1:F:414:ARG:NH1	1.87	1.07
1:D:259:ARG:HB2	1:E:170:SER:O	1.52	1.07
1:E:168:ILE:HG13	1:E:169:GLU:H	1.10	1.06
1:F:52:MET:HG3	1:F:62:VAL:HG11	1.37	1.05
1:A:174:ASN:N	1:A:174:ASN:OD1	1.63	1.05
1:A:315:ASP:O	1:A:316:TYR:HB2	1.54	1.05
1:C:299:ARG:NH2	1:D:31:LYS:HB3	1.73	1.03
1:F:315:ASP:O	1:F:316:TYR:HB2	1.58	1.02
1:C:315:ASP:O	1:C:316:TYR:HB2	1.57	1.02
1:D:315:ASP:O	1:D:316:TYR:HB2	1.59	1.02
1:A:190:TYR:OH	1:F:256:ALA:HB2	1.58	1.02
1:B:315:ASP:O	1:B:316:TYR:HB2	1.57	1.01
1:E:52:MET:HG3	1:E:62:VAL:HG11	1.43	1.00
1:C:52:MET:HG3	1:C:62:VAL:HG11	1.44	0.99
1:C:258:ARG:HG2	1:D:168:ILE:CG2	1.91	0.99
1:E:315:ASP:O	1:E:316:TYR:HB2	1.58	0.99
1:A:232:GLU:OE2	1:B:414:ARG:NH1	1.97	0.97
1:E:239:ILE:CD1	1:F:161:LEU:HG	1.94	0.96
1:E:157:ILE:HG13	1:E:158:ASP:H	1.31	0.95
1:C:299:ARG:HH22	1:D:31:LYS:HB3	1.27	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:ILE:HD13	1:F:161:LEU:HG	1.46	0.94
1:E:377:SER:HB2	1:E:380:LEU:HB2	1.48	0.94
1:A:157:ILE:HG23	1:A:158:ASP:H	1.29	0.94
1:B:52:MET:HG3	1:B:62:VAL:HG11	1.46	0.94
1:D:377:SER:HB2	1:D:380:LEU:HB2	1.50	0.93
1:A:257:ALA:HA	1:B:173:GLY:HA2	1.51	0.93
1:C:377:SER:HB2	1:C:380:LEU:HB2	1.50	0.93
1:A:377:SER:HB2	1:A:380:LEU:HB2	1.50	0.92
1:B:377:SER:HB2	1:B:380:LEU:HB2	1.51	0.91
1:F:377:SER:HB2	1:F:380:LEU:HB2	1.53	0.90
1:C:258:ARG:HH22	1:C:265:ASP:HB2	1.39	0.88
1:E:168:ILE:HG13	1:E:169:GLU:N	1.89	0.87
1:F:317:LEU:HD21	1:F:380:LEU:HD21	1.56	0.87
1:A:258:ARG:HG2	1:B:168:ILE:HG23	1.54	0.87
1:E:18:ALA:HB2	1:F:65:THR:HG21	1.59	0.84
1:A:258:ARG:HH22	1:A:265:ASP:HB2	1.43	0.84
1:A:157:ILE:HG23	1:A:158:ASP:N	1.93	0.83
1:E:317:LEU:HD21	1:E:380:LEU:HD21	1.59	0.83
1:A:52:MET:HG3	1:A:62:VAL:HG11	1.60	0.82
1:D:273:ILE:HG23	1:E:161:LEU:HD11	1.61	0.82
1:E:157:ILE:HG13	1:E:158:ASP:N	1.95	0.82
1:D:317:LEU:HD21	1:D:380:LEU:HD21	1.62	0.82
1:F:258:ARG:HH22	1:F:265:ASP:HB2	1.44	0.82
1:C:317:LEU:HD21	1:C:380:LEU:HD21	1.60	0.81
1:D:52:MET:HG3	1:D:62:VAL:CG1	2.10	0.81
1:E:52:MET:HG3	1:E:62:VAL:CG1	2.10	0.81
1:B:258:ARG:HH22	1:B:265:ASP:HB2	1.46	0.81
1:B:317:LEU:HD21	1:B:380:LEU:HD21	1.63	0.80
1:D:258:ARG:HH22	1:D:265:ASP:HB2	1.43	0.80
1:A:75:LEU:N	1:A:76:PRO:HD2	1.97	0.79
1:E:75:LEU:N	1:E:76:PRO:HD2	1.98	0.79
1:E:258:ARG:HH22	1:E:265:ASP:HB2	1.48	0.78
1:B:174:ASN:OD1	1:B:174:ASN:N	2.17	0.78
1:F:157:ILE:HG13	1:F:158:ASP:N	1.99	0.77
1:A:317:LEU:HD21	1:A:380:LEU:HD21	1.66	0.77
1:C:356:GLN:NE2	1:D:379:GLN:OE1	2.16	0.77
1:F:193:LYS:O	1:F:350:VAL:HG22	1.84	0.77
1:B:52:MET:HG3	1:B:62:VAL:CG1	2.15	0.77
1:D:124:VAL:HG12	1:E:110:LYS:HG3	1.67	0.76
1:C:229:HIS:HD2	1:C:289:GLN:OE1	1.67	0.75
1:A:190:TYR:OH	1:F:256:ALA:CB	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MET:HG3	1:A:62:VAL:CG1	2.15	0.75
1:E:229:HIS:HD2	1:E:289:GLN:OE1	1.70	0.74
1:B:392:ARG:HG3	1:B:406:VAL:HG22	1.67	0.74
1:B:36:THR:H	1:B:39:HIS:CD2	2.06	0.74
1:F:229:HIS:HD2	1:F:289:GLN:OE1	1.70	0.73
1:C:175:ILE:HD12	1:C:175:ILE:H	1.51	0.73
1:E:168:ILE:CG1	1:E:169:GLU:H	1.95	0.73
1:F:52:MET:HG3	1:F:62:VAL:CG1	2.18	0.73
1:D:75:LEU:N	1:D:76:PRO:HD2	2.03	0.73
1:B:256:ALA:O	1:C:171:ALA:HB1	1.89	0.72
1:E:273:ILE:HG23	1:F:165:TYR:CE2	2.24	0.72
1:F:158:ASP:OD1	1:F:161:LEU:HD13	1.89	0.72
1:F:75:LEU:N	1:F:76:PRO:HD2	2.05	0.72
1:B:193:LYS:O	1:B:350:VAL:HG22	1.89	0.72
1:F:406:VAL:HG23	1:F:425:PHE:HB2	1.72	0.72
1:A:392:ARG:HG3	1:A:406:VAL:HG22	1.69	0.72
1:D:259:ARG:HG2	1:E:171:ALA:HB2	1.71	0.72
1:E:52:MET:CG	1:E:62:VAL:HG11	2.19	0.72
1:E:392:ARG:HG3	1:E:406:VAL:HG22	1.71	0.72
1:D:107:TYR:O	1:D:111:ARG:HG3	1.90	0.72
1:A:22:SER:N	1:A:91:VAL:HG21	2.05	0.72
1:A:229:HIS:HD2	1:A:289:GLN:OE1	1.73	0.71
1:A:52:MET:CG	1:A:62:VAL:HG11	2.20	0.71
1:A:193:LYS:O	1:A:350:VAL:HG22	1.89	0.71
1:D:193:LYS:O	1:D:350:VAL:HG22	1.90	0.71
1:B:231:LEU:H	1:B:231:LEU:HD12	1.56	0.71
1:E:193:LYS:O	1:E:350:VAL:HG22	1.91	0.71
1:A:333:ILE:HG21	1:A:377:SER:HB3	1.73	0.71
1:B:110:LYS:HG3	1:C:124:VAL:HG11	1.71	0.71
1:C:75:LEU:N	1:C:76:PRO:HD2	2.05	0.70
1:C:193:LYS:O	1:C:350:VAL:HG22	1.92	0.70
1:C:52:MET:HG3	1:C:62:VAL:CG1	2.19	0.70
1:A:254:ILE:HG13	1:B:168:ILE:HD12	1.73	0.70
1:C:281:ILE:O	1:D:157:ILE:HG23	1.91	0.69
1:C:392:ARG:HG3	1:C:406:VAL:HG22	1.73	0.69
1:E:232:GLU:CD	1:F:414:ARG:HD3	2.11	0.69
1:B:75:LEU:N	1:B:76:PRO:HD2	2.08	0.69
1:D:229:HIS:HD2	1:D:289:GLN:OE1	1.75	0.69
1:F:107:TYR:O	1:F:111:ARG:HG3	1.93	0.68
1:A:231:LEU:H	1:A:231:LEU:HD12	1.58	0.68
1:E:239:ILE:HD11	1:F:161:LEU:HG	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:O	1:A:28:GLU:N	2.26	0.68
1:D:124:VAL:CG1	1:E:110:LYS:HG3	2.23	0.68
1:B:124:VAL:HG11	1:C:110:LYS:HG3	1.74	0.68
1:B:362:GLU:HB2	1:C:372:SER:HB3	1.76	0.68
1:E:158:ASP:O	1:E:160:ALA:N	2.24	0.67
1:E:377:SER:HB2	1:E:380:LEU:CB	2.24	0.67
1:D:392:ARG:HG3	1:D:406:VAL:HG22	1.74	0.67
1:C:119:GLN:HG3	1:C:123:ASN:ND2	2.10	0.67
1:A:157:ILE:CG2	1:A:158:ASP:H	2.07	0.67
1:E:231:LEU:H	1:E:231:LEU:HD12	1.60	0.67
1:F:315:ASP:O	1:F:316:TYR:CB	2.41	0.67
1:E:392:ARG:CG	1:E:406:VAL:HG22	2.25	0.66
1:A:377:SER:HB2	1:A:380:LEU:CB	2.25	0.66
1:A:406:VAL:HG23	1:A:425:PHE:HB2	1.76	0.66
1:C:231:LEU:HD12	1:C:231:LEU:H	1.60	0.66
1:D:377:SER:HB2	1:D:380:LEU:CB	2.26	0.66
1:F:231:LEU:H	1:F:231:LEU:HD12	1.61	0.66
1:C:315:ASP:O	1:C:316:TYR:CB	2.41	0.66
1:B:406:VAL:HG23	1:B:425:PHE:HB2	1.78	0.66
1:C:258:ARG:HG2	1:D:168:ILE:HG22	1.78	0.65
1:B:48:ILE:O	1:B:52:MET:HB2	1.97	0.65
1:D:406:VAL:HG23	1:D:425:PHE:HB2	1.77	0.65
1:D:52:MET:CG	1:D:62:VAL:HG11	2.17	0.65
1:E:48:ILE:O	1:E:52:MET:HB2	1.96	0.65
1:A:124:VAL:HG11	1:F:110:LYS:HG3	1.79	0.65
1:A:161:LEU:HD11	1:F:273:ILE:HG23	1.78	0.65
1:F:124:VAL:HG13	1:F:134:PRO:HB3	1.78	0.65
1:E:23:ILE:HG21	1:E:30:ILE:HG23	1.79	0.65
1:B:119:GLN:HG3	1:B:123:ASN:ND2	2.11	0.64
1:E:315:ASP:O	1:E:316:TYR:CB	2.41	0.64
1:E:273:ILE:HG23	1:F:165:TYR:HE2	1.60	0.64
1:F:392:ARG:HG3	1:F:406:VAL:HG22	1.79	0.64
1:A:36:THR:H	1:A:39:HIS:CD2	2.14	0.64
1:C:392:ARG:CG	1:C:406:VAL:HG22	2.28	0.64
1:B:167:GLU:O	1:B:171:ALA:HB2	1.96	0.64
1:C:406:VAL:HG23	1:C:425:PHE:HB2	1.77	0.64
1:F:377:SER:HB2	1:F:380:LEU:CB	2.27	0.64
1:F:257:ALA:HB1	1:F:261:PHE:CB	2.27	0.64
1:E:406:VAL:HG23	1:E:425:PHE:HB2	1.79	0.64
1:D:273:ILE:CG2	1:E:161:LEU:HD11	2.27	0.64
1:D:392:ARG:CG	1:D:406:VAL:HG22	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:GLN:HG3	1:F:123:ASN:ND2	2.12	0.64
1:A:137:GLU:O	1:A:141:GLU:HG2	1.98	0.63
1:F:36:THR:H	1:F:39:HIS:CD2	2.15	0.63
1:A:315:ASP:O	1:A:316:TYR:CB	2.40	0.62
1:B:175:ILE:H	1:B:175:ILE:HD12	1.64	0.62
1:B:107:TYR:O	1:B:111:ARG:HG3	2.00	0.62
1:D:119:GLN:HG3	1:D:123:ASN:ND2	2.15	0.62
1:B:124:VAL:HG13	1:B:134:PRO:HB3	1.82	0.62
1:C:356:GLN:HE22	1:D:379:GLN:CD	2.02	0.62
1:D:333:ILE:HG21	1:D:377:SER:HB3	1.82	0.61
1:A:154:ASP:HB3	1:F:300:GLN:HE22	1.65	0.61
1:F:316:TYR:HB3	1:F:319:LEU:HB2	1.81	0.61
1:C:258:ARG:HG2	1:D:168:ILE:HG23	1.81	0.61
1:E:333:ILE:HG21	1:E:377:SER:HB3	1.81	0.61
1:C:137:GLU:O	1:C:141:GLU:HG2	2.00	0.61
1:B:229:HIS:HD2	1:B:289:GLN:OE1	1.83	0.61
1:C:174:ASN:O	1:C:175:ILE:C	2.39	0.61
1:A:110:LYS:HG3	1:F:124:VAL:HG11	1.82	0.61
1:C:36:THR:H	1:C:39:HIS:CD2	2.18	0.61
1:F:333:ILE:HG21	1:F:377:SER:HB3	1.83	0.61
1:F:157:ILE:CG1	1:F:158:ASP:N	2.63	0.61
1:A:37:PRO:HB2	1:A:46:PHE:CE1	2.36	0.60
1:D:375:ARG:HE	1:D:376:GLU:HG3	1.65	0.60
1:D:36:THR:H	1:D:39:HIS:CD2	2.18	0.60
1:D:231:LEU:HD12	1:D:231:LEU:H	1.65	0.60
1:D:257:ALA:HB1	1:D:261:PHE:CB	2.31	0.60
1:C:107:TYR:O	1:C:111:ARG:HG3	2.01	0.60
1:B:259:ARG:H	1:C:171:ALA:HB3	1.66	0.60
1:C:317:LEU:CD2	1:C:380:LEU:HD21	2.29	0.60
1:C:203:ARG:NH2	1:D:381:GLU:OE1	2.32	0.60
1:E:255:LYS:HG2	1:F:190:TYR:CD1	2.37	0.60
1:A:26:GLU:C	1:A:28:GLU:H	2.04	0.60
1:A:190:TYR:HH	1:F:256:ALA:HB2	1.67	0.59
1:A:157:ILE:CG2	1:A:158:ASP:N	2.65	0.59
1:A:124:VAL:HG13	1:A:134:PRO:HB3	1.83	0.59
1:A:48:ILE:O	1:A:52:MET:HB2	2.02	0.59
1:B:52:MET:CG	1:B:62:VAL:HG11	2.27	0.59
1:B:392:ARG:CG	1:B:406:VAL:HG22	2.33	0.59
1:D:357:LEU:HD13	1:D:369:PRO:HB3	1.85	0.59
1:B:154:ASP:OD1	1:B:155:GLY:N	2.34	0.59
1:C:48:ILE:O	1:C:52:MET:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:VAL:O	1:A:168:ILE:HG12	2.02	0.59
1:B:377:SER:HB2	1:B:380:LEU:CB	2.30	0.59
1:F:41:SER:HB3	1:F:42:PRO:HD2	1.84	0.59
1:C:172:ASP:O	1:C:174:ASN:N	2.35	0.59
1:B:333:ILE:HG21	1:B:377:SER:HB3	1.84	0.58
1:A:119:GLN:HG3	1:A:123:ASN:ND2	2.18	0.58
1:A:357:LEU:HD13	1:A:369:PRO:HB3	1.85	0.58
1:C:356:GLN:CD	1:D:382:GLN:OE1	2.42	0.58
1:E:317:LEU:CD2	1:E:380:LEU:HD21	2.32	0.58
1:D:98:LYS:HE2	1:D:98:LYS:HA	1.84	0.58
1:B:316:TYR:HB3	1:B:319:LEU:HB2	1.85	0.58
1:C:377:SER:HB2	1:C:380:LEU:CB	2.28	0.58
1:C:257:ALA:HB1	1:C:261:PHE:CB	2.34	0.57
1:A:75:LEU:N	1:A:76:PRO:CD	2.67	0.57
1:E:12:ASN:HD21	1:F:69:ALA:HA	1.69	0.57
1:C:254:ILE:HA	1:C:258:ARG:HB2	1.86	0.57
1:C:333:ILE:HG21	1:C:377:SER:HB3	1.85	0.57
1:F:317:LEU:CD2	1:F:380:LEU:HD21	2.30	0.57
1:B:305:ASN:HB3	1:B:308:LYS:HD2	1.85	0.57
1:A:316:TYR:HB3	1:A:319:LEU:HB2	1.87	0.57
1:F:392:ARG:CG	1:F:406:VAL:HG22	2.33	0.57
1:B:22:SER:N	1:B:91:VAL:HG21	2.19	0.57
1:E:36:THR:H	1:E:39:HIS:CD2	2.22	0.57
1:C:316:TYR:HB3	1:C:319:LEU:HB2	1.87	0.57
1:D:316:TYR:HB3	1:D:319:LEU:HB2	1.87	0.57
1:D:22:SER:N	1:D:91:VAL:HG21	2.19	0.57
1:C:16:GLU:OE2	1:C:40:PHE:HA	2.05	0.57
1:A:258:ARG:CG	1:B:168:ILE:HG23	2.32	0.57
1:E:254:ILE:HA	1:E:258:ARG:HB2	1.85	0.57
1:B:37:PRO:HB2	1:B:46:PHE:CE1	2.39	0.57
1:D:48:ILE:O	1:D:52:MET:HB2	2.04	0.56
1:B:124:VAL:CG1	1:C:110:LYS:HG3	2.35	0.56
1:F:375:ARG:HE	1:F:376:GLU:HG3	1.70	0.56
1:A:236:LYS:NZ	1:B:163:THR:HG21	2.20	0.56
1:D:305:ASN:HB3	1:D:308:LYS:HD2	1.88	0.56
1:B:375:ARG:HE	1:B:376:GLU:HG3	1.71	0.56
1:F:254:ILE:HG23	1:F:255:LYS:H	1.71	0.56
1:C:22:SER:N	1:C:91:VAL:HG21	2.20	0.56
1:A:254:ILE:HA	1:A:258:ARG:HB2	1.88	0.56
1:A:254:ILE:HG13	1:B:168:ILE:CD1	2.34	0.56
1:C:299:ARG:NH1	1:C:299:ARG:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:GLN:HG3	1:E:123:ASN:ND2	2.20	0.56
1:C:299:ARG:NH1	1:D:31:LYS:O	2.39	0.56
1:F:378:GLY:C	1:F:380:LEU:H	2.09	0.56
1:C:375:ARG:HE	1:C:376:GLU:HG3	1.71	0.56
1:E:357:LEU:HD13	1:E:369:PRO:HB3	1.87	0.56
1:A:364:ARG:HD2	1:F:359:ARG:CZ	2.35	0.55
1:E:316:TYR:HB3	1:E:319:LEU:HB2	1.87	0.55
1:E:158:ASP:C	1:E:160:ALA:H	2.08	0.55
1:B:157:ILE:O	1:B:161:LEU:N	2.34	0.55
1:E:305:ASN:HB3	1:E:308:LYS:HD2	1.89	0.55
1:B:315:ASP:O	1:B:316:TYR:CB	2.41	0.55
1:C:282:ASN:HA	1:D:157:ILE:HG23	1.89	0.55
1:B:257:ALA:HB1	1:B:261:PHE:CB	2.36	0.55
1:F:254:ILE:O	1:F:255:LYS:C	2.44	0.55
1:D:317:LEU:CD2	1:D:380:LEU:HD21	2.35	0.55
1:B:254:ILE:HA	1:B:258:ARG:HB2	1.89	0.55
1:B:165:TYR:O	1:B:168:ILE:N	2.36	0.55
1:B:254:ILE:HG13	1:C:168:ILE:HG23	1.89	0.55
1:C:357:LEU:HD13	1:C:369:PRO:HB3	1.88	0.55
1:D:424:ALA:HB3	1:D:433:VAL:HB	1.89	0.54
1:A:392:ARG:CG	1:A:406:VAL:HG22	2.36	0.54
1:A:254:ILE:HG23	1:A:255:LYS:H	1.72	0.54
1:B:317:LEU:CD2	1:B:380:LEU:HD21	2.35	0.54
1:A:254:ILE:O	1:A:255:LYS:C	2.46	0.54
1:D:254:ILE:HG23	1:D:255:LYS:H	1.73	0.54
1:A:392:ARG:HH21	1:A:427:LYS:HE2	1.73	0.54
1:A:375:ARG:HE	1:A:376:GLU:HG3	1.72	0.54
1:D:315:ASP:O	1:D:316:TYR:CB	2.42	0.54
1:B:165:TYR:O	1:B:168:ILE:HG12	2.08	0.54
1:E:99:GLN:HE22	1:F:61:SER:H	1.54	0.54
1:F:23:ILE:HG21	1:F:30:ILE:HG23	1.89	0.54
1:E:75:LEU:N	1:E:76:PRO:CD	2.69	0.54
1:F:37:PRO:HB2	1:F:46:PHE:CE1	2.42	0.54
1:F:357:LEU:HD13	1:F:369:PRO:HB3	1.90	0.54
1:C:172:ASP:C	1:C:174:ASN:H	2.09	0.54
1:F:48:ILE:O	1:F:52:MET:HB2	2.08	0.54
1:B:229:HIS:CD2	1:B:294:ILE:HG12	2.43	0.54
1:D:201:ALA:O	1:D:389:PHE:HA	2.07	0.54
1:E:424:ALA:HB3	1:E:433:VAL:HB	1.90	0.53
1:E:162:VAL:O	1:E:165:TYR:HB2	2.08	0.53
1:C:52:MET:CG	1:C:62:VAL:HG11	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ILE:HG21	1:D:30:ILE:HG23	1.89	0.53
1:C:392:ARG:HH21	1:C:427:LYS:HE2	1.72	0.53
1:B:357:LEU:HD13	1:B:369:PRO:HB3	1.90	0.53
1:C:96:THR:HG22	1:D:61:SER:OG	2.09	0.53
1:A:138:ALA:O	1:A:142:LEU:HB2	2.08	0.53
1:F:316:TYR:HD2	1:F:319:LEU:HD13	1.73	0.53
1:A:317:LEU:CD2	1:A:380:LEU:HD21	2.36	0.53
1:F:137:GLU:O	1:F:141:GLU:HG2	2.09	0.53
1:C:378:GLY:C	1:C:380:LEU:H	2.12	0.53
1:A:27:PRO:HB3	1:A:62:VAL:O	2.08	0.53
1:A:424:ALA:HB3	1:A:433:VAL:HB	1.91	0.53
1:E:107:TYR:O	1:E:111:ARG:HG3	2.08	0.53
1:A:378:GLY:C	1:A:380:LEU:H	2.11	0.53
1:A:257:ALA:HB1	1:A:261:PHE:CB	2.39	0.53
1:D:161:LEU:O	1:D:161:LEU:HD23	2.08	0.53
1:B:392:ARG:HH21	1:B:427:LYS:HE2	1.72	0.53
1:E:257:ALA:HB1	1:E:261:PHE:CB	2.39	0.53
1:D:254:ILE:O	1:D:255:LYS:C	2.47	0.53
1:C:305:ASN:HB3	1:C:308:LYS:HD2	1.90	0.53
1:F:305:ASN:HB3	1:F:308:LYS:HD2	1.91	0.53
1:B:316:TYR:HD2	1:B:319:LEU:HD13	1.74	0.52
1:D:378:GLY:C	1:D:380:LEU:H	2.12	0.52
1:E:282:ASN:HA	1:F:157:ILE:HB	1.89	0.52
1:F:52:MET:CG	1:F:62:VAL:HG11	2.24	0.52
1:B:165:TYR:O	1:B:166:GLU:C	2.47	0.52
1:A:99:GLN:HE22	1:B:61:SER:H	1.57	0.52
1:C:115:SER:O	1:C:119:GLN:HB2	2.09	0.52
1:B:156:SER:C	1:B:157:ILE:HG13	2.29	0.52
1:F:150:THR:O	1:F:151:ASP:HB3	2.09	0.52
1:A:41:SER:HB3	1:A:42:PRO:HD2	1.91	0.52
1:A:160:ALA:O	1:A:164:VAL:HG23	2.10	0.52
1:B:259:ARG:NH1	1:C:169:GLU:HG2	2.24	0.52
1:E:392:ARG:HH21	1:E:427:LYS:HE2	1.74	0.52
1:D:157:ILE:HG13	1:D:157:ILE:O	2.09	0.52
1:B:201:ALA:O	1:B:389:PHE:HA	2.10	0.52
1:F:123:ASN:HB3	1:F:137:GLU:OE1	2.09	0.52
1:B:254:ILE:O	1:B:255:LYS:C	2.48	0.52
1:F:392:ARG:HH21	1:F:427:LYS:HE2	1.73	0.52
1:A:362:GLU:HB2	1:B:372:SER:HB3	1.91	0.52
1:C:41:SER:HB3	1:C:42:PRO:HD2	1.91	0.52
1:E:115:SER:O	1:E:119:GLN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:GLU:HG3	1:D:341:LYS:HE2	1.91	0.52
1:F:16:GLU:OE2	1:F:40:PHE:HA	2.10	0.52
1:A:93:SER:C	1:A:95:THR:H	2.14	0.51
1:C:254:ILE:O	1:C:255:LYS:C	2.48	0.51
1:E:316:TYR:HD2	1:E:319:LEU:HD13	1.75	0.51
1:C:175:ILE:HD12	1:C:175:ILE:N	2.21	0.51
1:D:392:ARG:HH21	1:D:427:LYS:HE2	1.75	0.51
1:E:254:ILE:O	1:E:255:LYS:C	2.49	0.51
1:B:64:PHE:N	1:B:64:PHE:CD1	2.78	0.51
1:B:134:PRO:HG3	1:C:110:LYS:HB2	1.92	0.51
1:E:386:ILE:HA	1:E:412:LYS:O	2.10	0.51
1:A:305:ASN:HB3	1:A:308:LYS:HD2	1.93	0.51
1:B:26:GLU:C	1:B:28:GLU:H	2.14	0.51
1:D:254:ILE:HA	1:D:258:ARG:HB2	1.93	0.51
1:A:16:GLU:OE2	1:A:40:PHE:HA	2.11	0.51
1:C:23:ILE:HG21	1:C:30:ILE:HG23	1.92	0.51
1:C:356:GLN:OE1	1:D:382:GLN:OE1	2.29	0.51
1:B:254:ILE:HG23	1:B:255:LYS:H	1.76	0.51
1:D:141:GLU:O	1:D:145:ILE:HG13	2.11	0.51
1:A:198:VAL:HG22	1:A:352:ILE:HG12	1.92	0.51
1:A:123:ASN:HB3	1:A:137:GLU:OE1	2.11	0.51
1:A:316:TYR:HD2	1:A:319:LEU:HD13	1.76	0.50
1:B:378:GLY:C	1:B:380:LEU:H	2.14	0.50
1:A:169:GLU:HB2	1:F:259:ARG:NH1	2.26	0.50
1:D:75:LEU:N	1:D:76:PRO:CD	2.73	0.50
1:D:16:GLU:OE2	1:D:40:PHE:HA	2.11	0.50
1:F:167:GLU:OE1	1:F:167:GLU:N	2.40	0.50
1:F:198:VAL:HG22	1:F:352:ILE:HG12	1.93	0.50
1:E:375:ARG:HE	1:E:376:GLU:HG3	1.75	0.50
1:B:435:LEU:O	1:B:436:GLU:HB2	2.11	0.50
1:A:371:LEU:HD11	1:A:411:ALA:HB1	1.94	0.50
1:E:254:ILE:HD11	1:F:168:ILE:HD12	1.94	0.50
1:A:146:GLU:C	1:A:148:SER:H	2.14	0.50
1:A:175:ILE:N	1:A:175:ILE:HD12	2.26	0.50
1:E:208:LYS:HD2	1:E:355:SER:O	2.11	0.50
1:B:110:LYS:HG3	1:C:124:VAL:CG1	2.41	0.50
1:A:256:ALA:O	1:B:171:ALA:HB1	2.11	0.50
1:A:115:SER:O	1:A:119:GLN:HB2	2.11	0.50
1:B:23:ILE:HG21	1:B:30:ILE:HG23	1.93	0.50
1:A:157:ILE:HD13	1:A:158:ASP:N	2.27	0.50
1:C:75:LEU:N	1:C:76:PRO:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ALA:HB3	1:C:433:VAL:HB	1.93	0.50
1:D:157:ILE:CG1	1:D:157:ILE:O	2.59	0.50
1:E:378:GLY:C	1:E:380:LEU:H	2.14	0.49
1:E:22:SER:N	1:E:91:VAL:HG21	2.26	0.49
1:A:364:ARG:HD2	1:F:359:ARG:NH2	2.27	0.49
1:B:115:SER:O	1:B:119:GLN:HB2	2.12	0.49
1:D:358:SER:HB2	1:D:375:ARG:HB2	1.94	0.49
1:B:137:GLU:O	1:B:141:GLU:HG2	2.13	0.49
1:D:316:TYR:HD2	1:D:319:LEU:HD13	1.78	0.49
1:F:75:LEU:N	1:F:76:PRO:CD	2.75	0.49
1:C:303:ARG:NH1	1:D:98:LYS:HD2	2.27	0.49
1:C:198:VAL:HG22	1:C:352:ILE:HG12	1.94	0.49
1:F:138:ALA:O	1:F:142:LEU:HB2	2.13	0.49
1:E:167:GLU:HA	1:E:170:SER:HB2	1.94	0.49
1:B:120:ILE:HG23	1:B:141:GLU:HG3	1.95	0.49
1:F:161:LEU:O	1:F:164:VAL:HG22	2.13	0.49
1:F:41:SER:O	1:F:46:PHE:HB2	2.12	0.48
1:B:16:GLU:OE2	1:B:40:PHE:HA	2.12	0.48
1:B:119:GLN:HG3	1:B:123:ASN:HD22	1.77	0.48
1:A:141:GLU:O	1:A:145:ILE:HG13	2.12	0.48
1:F:280:ASN:HD22	1:F:280:ASN:N	2.11	0.48
1:F:64:PHE:CD1	1:F:64:PHE:N	2.82	0.48
1:D:20:LEU:O	1:D:24:LEU:HG	2.14	0.48
1:F:22:SER:N	1:F:91:VAL:HG21	2.28	0.48
1:D:338:ARG:HG3	1:D:379:GLN:HG2	1.95	0.48
1:B:239:ILE:HG21	1:C:161:LEU:HG	1.96	0.48
1:F:217:LYS:O	1:F:220:SER:N	2.47	0.48
1:C:120:ILE:O	1:C:124:VAL:HG23	2.14	0.48
1:B:258:ARG:HB3	1:C:171:ALA:CB	2.44	0.48
1:E:337:SER:HB2	1:E:380:LEU:HD22	1.95	0.48
1:E:142:LEU:O	1:E:146:GLU:HG3	2.14	0.48
1:B:386:ILE:HA	1:B:412:LYS:O	2.14	0.48
1:F:406:VAL:HG23	1:F:425:PHE:CB	2.42	0.48
1:D:359:ARG:NH1	1:E:366:ASP:HB3	2.29	0.48
1:F:337:SER:HB2	1:F:380:LEU:HD22	1.96	0.48
1:B:362:GLU:HB2	1:C:372:SER:CB	2.41	0.48
1:A:356:GLN:HE22	1:B:382:GLN:CD	2.17	0.48
1:F:125:ASN:OD1	1:F:125:ASN:N	2.46	0.48
1:E:282:ASN:ND2	1:F:157:ILE:HD13	2.29	0.47
1:B:116:ILE:HG12	1:B:144:GLU:HB3	1.95	0.47
1:A:157:ILE:HD13	1:A:158:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LEU:O	1:C:146:GLU:HG3	2.14	0.47
1:E:239:ILE:HD11	1:F:161:LEU:CG	2.43	0.47
1:A:414:ARG:O	1:F:237:GLU:OE1	2.32	0.47
1:D:26:GLU:C	1:D:28:GLU:H	2.17	0.47
1:B:175:ILE:HD12	1:B:175:ILE:N	2.28	0.47
1:A:31:LYS:HE3	1:A:56:ASP:OD1	2.14	0.47
1:E:241:ARG:HH21	1:F:415:ASP:HA	1.79	0.47
1:F:424:ALA:HB3	1:F:433:VAL:HB	1.95	0.47
1:B:337:SER:HB2	1:B:380:LEU:HD22	1.95	0.47
1:F:257:ALA:O	1:F:259:ARG:N	2.48	0.47
1:A:313:MET:HA	1:A:352:ILE:O	2.14	0.47
1:A:386:ILE:HA	1:A:412:LYS:O	2.15	0.47
1:C:26:GLU:C	1:C:28:GLU:H	2.18	0.47
1:E:316:TYR:CD2	1:E:319:LEU:HD13	2.49	0.47
1:F:358:SER:HB2	1:F:375:ARG:HB2	1.95	0.47
1:E:282:ASN:ND2	1:F:157:ILE:CD1	2.78	0.47
1:A:229:HIS:CD2	1:A:294:ILE:HG12	2.50	0.47
1:D:316:TYR:CD2	1:D:319:LEU:HD13	2.49	0.47
1:F:254:ILE:HA	1:F:258:ARG:HB2	1.97	0.47
1:A:269:LEU:C	1:A:271:MET:H	2.17	0.47
1:B:316:TYR:CD2	1:B:319:LEU:HD13	2.50	0.46
1:A:152:ASP:N	1:A:152:ASP:OD1	2.48	0.46
1:E:160:ALA:O	1:E:164:VAL:N	2.42	0.46
1:A:142:LEU:O	1:A:146:GLU:HG3	2.14	0.46
1:B:138:ALA:O	1:B:142:LEU:HB2	2.15	0.46
1:C:410:ILE:HD12	1:C:410:ILE:N	2.31	0.46
1:C:201:ALA:O	1:C:389:PHE:HA	2.16	0.46
1:E:44:LYS:O	1:E:48:ILE:HG12	2.15	0.46
1:B:75:LEU:N	1:B:76:PRO:CD	2.76	0.46
1:C:358:SER:HB2	1:C:375:ARG:HB2	1.98	0.46
1:E:157:ILE:CG1	1:E:158:ASP:N	2.70	0.46
1:B:368:ARG:HA	1:B:369:PRO:HD3	1.77	0.46
1:C:99:GLN:HE22	1:D:61:SER:H	1.64	0.46
1:F:174:ASN:O	1:F:175:ILE:O	2.34	0.46
1:F:316:TYR:CD2	1:F:319:LEU:HD13	2.50	0.46
1:A:259:ARG:HB3	1:B:171:ALA:O	2.16	0.46
1:F:254:ILE:O	1:F:258:ARG:HB2	2.16	0.46
1:A:217:LYS:O	1:A:220:SER:N	2.49	0.46
1:E:406:VAL:HG23	1:E:425:PHE:CB	2.45	0.46
1:D:406:VAL:HG23	1:D:425:PHE:CB	2.45	0.46
1:C:41:SER:O	1:C:46:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:CD1	1:A:64:PHE:N	2.84	0.46
1:E:362:GLU:HB2	1:F:372:SER:HB3	1.97	0.46
1:A:239:ILE:HD13	1:B:161:LEU:HD22	1.97	0.46
1:E:368:ARG:HA	1:E:369:PRO:HD3	1.79	0.45
1:E:137:GLU:O	1:E:141:GLU:HG2	2.16	0.45
1:F:257:ALA:HB1	1:F:261:PHE:HB2	1.98	0.45
1:E:229:HIS:CD2	1:E:294:ILE:HG12	2.52	0.45
1:A:12:ASN:HD21	1:B:69:ALA:HA	1.81	0.45
1:C:254:ILE:HG23	1:C:255:LYS:H	1.81	0.45
1:B:258:ARG:HB3	1:C:171:ALA:HB2	1.97	0.45
1:E:254:ILE:HG23	1:E:255:LYS:H	1.81	0.45
1:C:208:LYS:HD2	1:C:355:SER:O	2.17	0.45
1:A:203:ARG:NH1	1:A:359:ARG:HA	2.31	0.45
1:D:41:SER:HB3	1:D:42:PRO:HD2	1.98	0.45
1:E:169:GLU:O	1:E:170:SER:O	2.35	0.45
1:E:172:ASP:N	1:E:172:ASP:OD2	2.50	0.45
1:B:406:VAL:HG23	1:B:425:PHE:CB	2.45	0.45
1:B:175:ILE:H	1:B:175:ILE:CD1	2.29	0.45
1:E:381:GLU:HA	1:E:387:ILE:HD11	1.98	0.45
1:C:299:ARG:HB3	1:C:299:ARG:HH11	1.82	0.45
1:D:435:LEU:O	1:D:436:GLU:C	2.55	0.45
1:E:356:GLN:OE1	1:F:382:GLN:HG2	2.17	0.45
1:F:254:ILE:HA	1:F:258:ARG:HD2	1.99	0.45
1:E:254:ILE:O	1:E:258:ARG:HB2	2.16	0.45
1:F:406:VAL:CG2	1:F:425:PHE:HB2	2.44	0.45
1:C:406:VAL:HG23	1:C:425:PHE:CB	2.45	0.45
1:E:175:ILE:N	1:E:175:ILE:HD12	2.31	0.45
1:E:26:GLU:C	1:E:28:GLU:H	2.20	0.45
1:C:367:LYS:HB2	1:C:391:TYR:HE1	1.82	0.44
1:F:212:ALA:HB1	1:F:313:MET:CE	2.46	0.44
1:F:257:ALA:O	1:F:258:ARG:C	2.55	0.44
1:D:119:GLN:HG3	1:D:123:ASN:HD22	1.81	0.44
1:E:138:ALA:O	1:E:142:LEU:HB2	2.17	0.44
1:A:39:HIS:HE1	1:A:151:ASP:OD2	2.01	0.44
1:A:357:LEU:CD1	1:A:369:PRO:HB3	2.46	0.44
1:A:236:LYS:HZ1	1:B:163:THR:HG21	1.82	0.44
1:A:152:ASP:HB2	1:A:153:ASP:H	1.52	0.44
1:D:237:GLU:CD	1:E:415:ASP:HA	2.37	0.44
1:D:386:ILE:HA	1:D:412:LYS:O	2.18	0.44
1:A:316:TYR:CD2	1:A:319:LEU:HD13	2.53	0.44
1:F:201:ALA:O	1:F:202:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ASN:HD22	1:E:280:ASN:N	2.14	0.44
1:D:44:LYS:O	1:D:48:ILE:HG12	2.17	0.44
1:B:258:ARG:HG2	1:C:168:ILE:O	2.16	0.44
1:D:368:ARG:HA	1:D:369:PRO:HD3	1.81	0.44
1:C:37:PRO:HB2	1:C:46:PHE:CE1	2.52	0.44
1:B:371:LEU:HD11	1:B:411:ALA:HB1	2.00	0.44
1:F:44:LYS:O	1:F:48:ILE:HG12	2.18	0.44
1:E:282:ASN:HD21	1:F:157:ILE:HD13	1.82	0.44
1:A:337:SER:HB2	1:A:380:LEU:HD22	1.99	0.44
1:A:212:ALA:HB2	1:A:354:LEU:HD11	2.00	0.44
1:A:201:ALA:O	1:A:389:PHE:HA	2.17	0.44
1:F:410:ILE:N	1:F:410:ILE:HD12	2.33	0.44
1:D:410:ILE:HD12	1:D:410:ILE:N	2.33	0.44
1:E:171:ALA:O	1:E:172:ASP:HB3	2.17	0.44
1:A:212:ALA:HB1	1:A:313:MET:CE	2.48	0.44
1:D:124:VAL:HG13	1:D:134:PRO:HB3	2.00	0.43
1:A:154:ASP:CB	1:F:300:GLN:HE22	2.30	0.43
1:F:201:ALA:O	1:F:389:PHE:HA	2.19	0.43
1:E:201:ALA:O	1:E:389:PHE:HA	2.17	0.43
1:C:280:ASN:N	1:C:280:ASN:HD22	2.16	0.43
1:F:161:LEU:HD23	1:F:161:LEU:O	2.18	0.43
1:A:406:VAL:CG2	1:A:425:PHE:HB2	2.47	0.43
1:A:178:VAL:O	1:A:191:GLY:HA2	2.18	0.43
1:A:30:ILE:HD12	1:A:31:LYS:H	1.83	0.43
1:C:254:ILE:HA	1:C:258:ARG:HD2	2.00	0.43
1:A:259:ARG:CB	1:B:171:ALA:O	2.67	0.43
1:F:146:GLU:C	1:F:148:SER:H	2.22	0.43
1:B:259:ARG:HB2	1:C:171:ALA:H	1.83	0.43
1:B:165:TYR:O	1:B:167:GLU:N	2.52	0.43
1:A:406:VAL:HG23	1:A:425:PHE:CB	2.44	0.43
1:E:410:ILE:HD12	1:E:410:ILE:N	2.33	0.43
1:F:158:ASP:HA	1:F:161:LEU:HB3	2.00	0.43
1:D:254:ILE:O	1:D:258:ARG:HB2	2.19	0.43
1:F:157:ILE:HG13	1:F:158:ASP:OD1	2.18	0.43
1:D:311:ILE:HG13	1:D:350:VAL:HB	2.00	0.43
1:C:368:ARG:HA	1:C:369:PRO:HD3	1.79	0.43
1:C:355:SER:OG	1:C:356:GLN:N	2.52	0.43
1:C:254:ILE:O	1:C:258:ARG:HB2	2.19	0.43
1:B:256:ALA:HB3	1:C:190:TYR:CE2	2.53	0.43
1:D:64:PHE:N	1:D:64:PHE:CD1	2.87	0.43
1:A:338:ARG:HG3	1:A:379:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ALA:HB1	1:B:313:MET:HE2	2.00	0.42
1:C:316:TYR:OH	1:D:382:GLN:HB3	2.18	0.42
1:E:161:LEU:O	1:E:164:VAL:HB	2.20	0.42
1:A:254:ILE:O	1:A:258:ARG:HB2	2.19	0.42
1:C:172:ASP:C	1:C:174:ASN:N	2.72	0.42
1:A:26:GLU:C	1:A:28:GLU:N	2.71	0.42
1:A:358:SER:HB2	1:A:375:ARG:HB2	2.00	0.42
1:A:198:VAL:CG2	1:A:352:ILE:HG12	2.49	0.42
1:C:262:ALA:HB1	1:C:265:ASP:OD2	2.19	0.42
1:C:337:SER:HB2	1:C:380:LEU:HD22	2.00	0.42
1:D:254:ILE:HA	1:D:258:ARG:HD2	2.00	0.42
1:F:119:GLN:HG3	1:F:123:ASN:HD22	1.84	0.42
1:E:119:GLN:HG3	1:E:123:ASN:HD22	1.84	0.42
1:D:402:SER:HB3	1:D:405:ILE:HB	2.02	0.42
1:B:367:LYS:HB2	1:B:391:TYR:HE1	1.85	0.42
1:E:367:LYS:HB2	1:E:391:TYR:HE1	1.85	0.42
1:C:25:THR:O	1:C:27:PRO:HD3	2.19	0.42
1:A:208:LYS:HD2	1:A:355:SER:O	2.19	0.42
1:D:367:LYS:HB2	1:D:391:TYR:HE1	1.84	0.42
1:A:52:MET:HG3	1:A:62:VAL:HG13	1.97	0.42
1:A:311:ILE:HD12	1:A:311:ILE:N	2.35	0.42
1:E:358:SER:HB2	1:E:375:ARG:HB2	2.01	0.42
1:D:229:HIS:CD2	1:D:294:ILE:HG12	2.54	0.42
1:C:257:ALA:O	1:C:259:ARG:N	2.53	0.42
1:E:257:ALA:O	1:E:259:ARG:N	2.53	0.42
1:D:145:ILE:O	1:D:145:ILE:HG22	2.20	0.42
1:C:154:ASP:CG	1:C:155:GLY:N	2.72	0.42
1:B:31:LYS:HE3	1:B:56:ASP:OD1	2.20	0.42
1:A:252:GLN:HG2	1:B:190:TYR:OH	2.19	0.42
1:A:171:ALA:O	1:A:172:ASP:C	2.59	0.42
1:E:173:GLY:O	1:E:174:ASN:CB	2.66	0.42
1:F:31:LYS:HE3	1:F:56:ASP:OD1	2.20	0.41
1:C:242:LEU:HB3	1:C:276:ILE:HD12	2.01	0.41
1:D:49:TYR:HA	1:D:52:MET:HB3	2.02	0.41
1:A:254:ILE:HA	1:A:258:ARG:HD2	2.02	0.41
1:A:292:ASN:HD22	1:B:31:LYS:HD3	1.85	0.41
1:F:26:GLU:C	1:F:28:GLU:H	2.23	0.41
1:E:41:SER:O	1:E:46:PHE:HB2	2.20	0.41
1:D:138:ALA:O	1:D:142:LEU:HB2	2.21	0.41
1:A:381:GLU:HA	1:A:387:ILE:HD11	2.02	0.41
1:D:406:VAL:CG2	1:D:425:PHE:HB2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ALA:HB1	1:A:313:MET:HE2	2.03	0.41
1:C:386:ILE:HA	1:C:412:LYS:O	2.20	0.41
1:B:49:TYR:HA	1:B:52:MET:HB3	2.02	0.41
1:D:115:SER:O	1:D:119:GLN:HB2	2.19	0.41
1:C:358:SER:C	1:C:360:GLN:H	2.24	0.41
1:F:368:ARG:HA	1:F:369:PRO:HD3	1.79	0.41
1:A:269:LEU:C	1:A:271:MET:N	2.74	0.41
1:E:198:VAL:HG22	1:E:352:ILE:HG12	2.01	0.41
1:F:269:LEU:C	1:F:271:MET:H	2.23	0.41
1:D:198:VAL:HG22	1:D:352:ILE:HG12	2.02	0.41
1:E:167:GLU:O	1:E:170:SER:HB2	2.20	0.41
1:A:311:ILE:HG13	1:A:350:VAL:HB	2.02	0.41
1:F:26:GLU:HB2	1:F:29:LEU:HD22	2.02	0.41
1:C:38:GLU:HG2	1:C:38:GLU:H	1.67	0.41
1:F:163:THR:O	1:F:167:GLU:OE1	2.39	0.41
1:C:138:ALA:O	1:C:142:LEU:HB2	2.20	0.41
1:D:221:ASP:C	1:D:223:ASP:H	2.24	0.41
1:A:150:THR:HG21	1:F:303:ARG:NH2	2.35	0.41
1:D:25:THR:O	1:D:27:PRO:HD3	2.21	0.41
1:C:49:TYR:HA	1:C:52:MET:HB3	2.03	0.41
1:A:262:ALA:HB1	1:A:265:ASP:OD2	2.19	0.41
1:A:358:SER:C	1:A:360:GLN:H	2.23	0.41
1:E:259:ARG:HB2	1:F:171:ALA:O	2.21	0.41
1:F:262:ALA:HB1	1:F:265:ASP:OD2	2.20	0.41
1:E:201:ALA:O	1:E:202:ALA:HB2	2.20	0.41
1:F:381:GLU:HA	1:F:387:ILE:HD11	2.02	0.41
1:C:269:LEU:C	1:C:271:MET:H	2.22	0.41
1:A:158:ASP:HA	1:A:161:LEU:HB2	2.03	0.41
1:A:178:VAL:HG21	1:A:311:ILE:HD11	2.03	0.41
1:B:63:ASP:O	1:B:64:PHE:C	2.58	0.41
1:A:12:ASN:O	1:A:16:GLU:HB2	2.21	0.41
1:A:201:ALA:O	1:A:202:ALA:HB2	2.20	0.41
1:B:146:GLU:C	1:B:148:SER:H	2.23	0.41
1:E:124:VAL:HG13	1:E:134:PRO:HB3	2.02	0.41
1:B:242:LEU:HB3	1:B:276:ILE:HD12	2.03	0.41
1:B:311:ILE:HD12	1:B:311:ILE:N	2.36	0.41
1:F:311:ILE:HD12	1:F:311:ILE:N	2.36	0.41
1:B:221:ASP:C	1:B:223:ASP:H	2.24	0.41
1:B:410:ILE:HD12	1:B:410:ILE:N	2.36	0.41
1:E:326:ASN:HD22	1:E:326:ASN:HA	1.67	0.41
1:B:215:GLN:O	1:B:219:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ARG:HD3	1:C:169:GLU:O	2.21	0.41
1:C:239:ILE:HD11	1:D:157:ILE:HD12	2.03	0.41
1:A:308:LYS:NZ	1:A:308:LYS:HB3	2.36	0.41
1:F:212:ALA:HB2	1:F:354:LEU:HD11	2.02	0.41
1:E:313:MET:HA	1:E:352:ILE:O	2.21	0.41
1:C:338:ARG:HG3	1:C:379:GLN:HG2	2.02	0.41
1:C:327:ASP:O	1:D:324:LYS:NZ	2.54	0.41
1:D:344:ALA:HB2	1:D:351:VAL:CG2	2.51	0.41
1:E:38:GLU:HG2	1:E:38:GLU:H	1.65	0.41
1:A:158:ASP:C	1:A:160:ALA:N	2.74	0.40
1:F:257:ALA:HB1	1:F:261:PHE:HB3	2.02	0.40
1:C:406:VAL:CG2	1:C:425:PHE:HB2	2.47	0.40
1:D:381:GLU:HA	1:D:387:ILE:HD11	2.03	0.40
1:A:367:LYS:HB2	1:A:391:TYR:HE1	1.86	0.40
1:F:340:LEU:HD23	1:F:340:LEU:HA	1.93	0.40
1:B:48:ILE:CD1	1:B:78:LEU:HB3	2.52	0.40
1:D:337:SER:HB2	1:D:380:LEU:HD22	2.03	0.40
1:B:313:MET:HA	1:B:352:ILE:O	2.21	0.40
1:F:49:TYR:HA	1:F:52:MET:HB3	2.02	0.40
1:C:273:ILE:HD13	1:D:165:TYR:CD2	2.57	0.40
1:E:254:ILE:HA	1:E:258:ARG:HD2	2.03	0.40
1:C:206:MET:CE	1:C:391:TYR:HA	2.52	0.40
1:D:212:ALA:HB2	1:D:354:LEU:HD11	2.04	0.40
1:F:244:VAL:HG12	1:F:244:VAL:O	2.20	0.40
1:F:299:ARG:NH1	1:F:299:ARG:HB3	2.37	0.40
1:C:347:LEU:HD12	1:C:347:LEU:HA	1.89	0.40
1:C:282:ASN:HA	1:D:157:ILE:CG2	2.52	0.40
1:B:154:ASP:CG	1:B:155:GLY:N	2.75	0.40
1:B:26:GLU:O	1:B:28:GLU:N	2.50	0.40
1:A:30:ILE:HD12	1:A:31:LYS:N	2.36	0.40
1:F:367:LYS:HB2	1:F:391:TYR:HE1	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/444 (94%)	359 (86%)	41 (10%)	15 (4%)	4	40
1	B	415/444 (94%)	357 (86%)	47 (11%)	11 (3%)	6	46
1	C	415/444 (94%)	365 (88%)	38 (9%)	12 (3%)	6	45
1	D	403/444 (91%)	355 (88%)	40 (10%)	8 (2%)	9	53
1	E	415/444 (94%)	358 (86%)	43 (10%)	14 (3%)	5	42
1	F	415/444 (94%)	354 (85%)	46 (11%)	15 (4%)	4	40
All	All	2478/2664 (93%)	2148 (87%)	255 (10%)	75 (3%)	5	44

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	157	ILE
1	A	255	LYS
1	A	258	ARG
1	A	316	TYR
1	A	375	ARG
1	B	44	LYS
1	B	166	GLU
1	B	255	LYS
1	B	258	ARG
1	B	316	TYR
1	B	375	ARG
1	C	44	LYS
1	C	175	ILE
1	C	255	LYS
1	C	258	ARG
1	C	316	TYR
1	C	375	ARG
1	D	44	LYS
1	D	255	LYS
1	D	258	ARG
1	D	316	TYR
1	D	375	ARG
1	E	165	TYR
1	E	168	ILE
1	E	170	SER
1	E	255	LYS

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Mol	Chain	Res	Type
1	E	258	ARG
1	E	316	TYR
1	E	375	ARG
1	F	151	ASP
1	F	175	ILE
1	F	255	LYS
1	F	258	ARG
1	F	316	TYR
1	F	375	ARG
1	B	157	ILE
1	B	193	LYS
1	C	173	GLY
1	C	193	LYS
1	D	193	LYS
1	E	44	LYS
1	E	159	GLU
1	E	166	GLU
1	E	172	ASP
1	E	193	LYS
1	F	44	LYS
1	F	154	ASP
1	F	173	GLY
1	A	70	ARG
1	A	94	THR
1	A	172	ASP
1	A	193	LYS
1	B	158	ASP
1	F	193	LYS
1	A	27	PRO
1	F	379	GLN
1	A	147	ALA
1	A	149	GLY
1	A	254	ILE
1	B	27	PRO
1	C	170	SER
1	C	379	GLN
1	D	379	GLN
1	F	153	ASP
1	F	159	GLU
1	A	379	GLN
1	B	153	ASP
1	C	27	PRO

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Mol	Chain	Res	Type
1	E	379	GLN
1	F	254	ILE
1	C	124	VAL
1	F	157	ILE
1	D	27	PRO
1	E	27	PRO

### 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	361/386 (94%)	348 (96%)	13 (4%)	42	76
1	B	361/386 (94%)	343 (95%)	18 (5%)	30	68
1	C	361/386 (94%)	350 (97%)	11 (3%)	48	79
1	D	354/386 (92%)	345 (98%)	9 (2%)	55	82
1	E	361/386 (94%)	346 (96%)	15 (4%)	36	72
1	F	361/386 (94%)	347 (96%)	14 (4%)	39	74
All	All	2159/2316 (93%)	2079 (96%)	80 (4%)	41	75

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	64	PHE
1	A	71	VAL
1	A	152	ASP
1	A	157	ILE
1	A	158	ASP
1	A	174	ASN
1	A	231	LEU
1	A	254	ILE
1	A	308	LYS
1	A	316	TYR
1	A	376	GLU

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Mol	Chain	Res	Type
1	A	380	LEU
1	B	30	ILE
1	B	64	PHE
1	B	101	CYS
1	B	144	GLU
1	B	157	ILE
1	B	161	LEU
1	B	165	TYR
1	B	166	GLU
1	B	174	ASN
1	B	231	LEU
1	B	254	ILE
1	B	308	LYS
1	B	316	TYR
1	B	319	LEU
1	B	348	ASP
1	B	368	ARG
1	B	376	GLU
1	B	380	LEU
1	C	30	ILE
1	C	64	PHE
1	C	144	GLU
1	C	166	GLU
1	C	174	ASN
1	C	231	LEU
1	C	254	ILE
1	C	308	LYS
1	C	316	TYR
1	C	376	GLU
1	C	380	LEU
1	D	30	ILE
1	D	64	PHE
1	D	165	TYR
1	D	167	GLU
1	D	231	LEU
1	D	308	LYS
1	D	316	TYR
1	D	376	GLU
1	D	380	LEU
1	E	30	ILE
1	E	64	PHE
1	E	144	GLU

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Mol	Chain	Res	Type
1	E	153	ASP
1	E	159	GLU
1	E	165	TYR
1	E	167	GLU
1	E	174	ASN
1	E	231	LEU
1	E	308	LYS
1	E	316	TYR
1	E	319	LEU
1	E	368	ARG
1	E	376	GLU
1	E	380	LEU
1	F	30	ILE
1	F	64	PHE
1	F	125	ASN
1	F	150	THR
1	F	157	ILE
1	F	174	ASN
1	F	198	VAL
1	F	231	LEU
1	F	308	LYS
1	F	316	TYR
1	F	319	LEU
1	F	348	ASP
1	F	376	GLU
1	F	380	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	45	HIS
1	A	77	GLN
1	A	100	HIS
1	A	102	GLN
1	A	109	GLN
1	A	119	GLN
1	A	123	ASN
1	A	196	ASN
1	A	215	GLN
1	A	229	HIS
1	A	280	ASN

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Mol	Chain	Res	Type
1	A	282	ASN
1	A	292	ASN
1	A	305	ASN
1	A	326	ASN
1	A	331	ASN
1	A	356	GLN
1	A	365	GLN
1	A	404	ASN
1	B	39	HIS
1	B	45	HIS
1	B	77	GLN
1	B	99	GLN
1	B	102	GLN
1	B	109	GLN
1	B	119	GLN
1	B	123	ASN
1	B	125	ASN
1	B	196	ASN
1	B	215	GLN
1	B	229	HIS
1	B	280	ASN
1	B	282	ASN
1	B	305	ASN
1	B	326	ASN
1	B	331	ASN
1	B	365	GLN
1	B	382	GLN
1	B	404	ASN
1	C	39	HIS
1	C	77	GLN
1	C	100	HIS
1	C	102	GLN
1	C	109	GLN
1	C	119	GLN
1	C	123	ASN
1	C	174	ASN
1	C	196	ASN
1	C	215	GLN
1	C	222	ASN
1	C	229	HIS
1	C	280	ASN
1	C	282	ASN

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Mol	Chain	Res	Type
1	C	305	ASN
1	C	326	ASN
1	C	331	ASN
1	C	356	GLN
1	C	365	GLN
1	C	404	ASN
1	D	39	HIS
1	D	45	HIS
1	D	77	GLN
1	D	99	GLN
1	D	102	GLN
1	D	109	GLN
1	D	119	GLN
1	D	123	ASN
1	D	196	ASN
1	D	215	GLN
1	D	222	ASN
1	D	229	HIS
1	D	280	ASN
1	D	282	ASN
1	D	305	ASN
1	D	326	ASN
1	D	331	ASN
1	D	365	GLN
1	D	379	GLN
1	D	404	ASN
1	E	39	HIS
1	E	77	GLN
1	E	100	HIS
1	E	102	GLN
1	E	109	GLN
1	E	119	GLN
1	E	123	ASN
1	E	196	ASN
1	E	215	GLN
1	E	222	ASN
1	E	229	HIS
1	E	252	GLN
1	E	280	ASN
1	E	282	ASN
1	E	305	ASN
1	E	326	ASN

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Mol	Chain	Res	Type
1	E	331	ASN
1	E	365	GLN
1	E	404	ASN
1	F	39	HIS
1	F	77	GLN
1	F	99	GLN
1	F	102	GLN
1	F	109	GLN
1	F	119	GLN
1	F	123	ASN
1	F	196	ASN
1	F	215	GLN
1	F	222	ASN
1	F	229	HIS
1	F	280	ASN
1	F	282	ASN
1	F	300	GLN
1	F	305	ASN
1	F	326	ASN
1	F	331	ASN
1	F	365	GLN
1	F	404	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	419/444 (94%)	0.61	30 (7%) 18 12	103, 118, 142, 151	0
1	B	419/444 (94%)	0.66	35 (8%) 14 10	103, 117, 142, 151	0
1	C	419/444 (94%)	1.43	121 (28%) 1 1	103, 117, 142, 151	0
1	D	409/444 (92%)	1.42	95 (23%) 1 1	103, 117, 142, 151	0
1	E	419/444 (94%)	1.43	113 (26%) 1 1	103, 117, 142, 151	0
1	F	419/444 (94%)	0.97	68 (16%) 3 3	103, 117, 142, 151	0
All	All	2504/2664 (93%)	1.08	462 (18%) 2 2	103, 117, 142, 151	0

All (462) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	263	SER	9.2
1	C	365	GLN	9.1
1	D	434	ASN	8.9
1	A	256	ALA	8.3
1	C	402	SER	8.2
1	F	365	GLN	7.3
1	D	435	LEU	7.1
1	C	271	MET	6.9
1	E	79	GLY	6.7
1	C	358	SER	6.7
1	B	399	GLU	6.4
1	A	255	LYS	6.2
1	F	363	GLN	6.2
1	F	159	GLU	5.8
1	E	174	ASN	5.8
1	B	152	ASP	5.7
1	E	376	GLU	5.7
1	C	400	SER	5.6
1	D	262	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	260	ASP	5.6
1	D	32	GLU	5.5
1	C	272	ALA	5.5
1	E	171	ALA	5.4
1	C	260	ASP	5.4
1	C	397	ASP	5.4
1	D	158	ASP	5.3
1	E	32	GLU	5.2
1	D	260	ASP	5.2
1	D	250	ASN	5.1
1	E	77	GLN	5.1
1	E	61	SER	5.1
1	E	134	PRO	5.1
1	D	366	ASP	5.0
1	D	308	LYS	4.9
1	E	280	ASN	4.9
1	C	279	SER	4.8
1	E	377	SER	4.8
1	F	364	ARG	4.8
1	F	252	GLN	4.7
1	E	119	GLN	4.7
1	E	375	ARG	4.7
1	E	250	ASN	4.6
1	E	401	GLU	4.5
1	C	267	GLY	4.4
1	C	141	GLU	4.4
1	F	90	SER	4.4
1	F	170	SER	4.4
1	E	260	ASP	4.4
1	E	158	ASP	4.4
1	D	113	ALA	4.4
1	D	179	PRO	4.3
1	E	78	LEU	4.3
1	E	223	ASP	4.3
1	E	172	ASP	4.3
1	D	306	PRO	4.3
1	E	100	HIS	4.3
1	F	12	ASN	4.3
1	C	58	LYS	4.2
1	E	72	GLY	4.2
1	F	260	ASP	4.2
1	C	326	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	157	ILE	4.2
1	D	399	GLU	4.1
1	C	398	LYS	4.1
1	C	403	LYS	4.0
1	E	166	GLU	4.0
1	E	251	ALA	4.0
1	D	303	ARG	4.0
1	C	134	PRO	4.0
1	F	358	SER	4.0
1	E	141	GLU	3.9
1	F	415	ASP	3.9
1	B	306	PRO	3.9
1	D	404	ASN	3.9
1	D	252	GLN	3.8
1	F	398	LYS	3.8
1	E	133	LYS	3.8
1	F	434	ASN	3.8
1	C	259	ARG	3.8
1	C	224	ASP	3.8
1	C	57	ARG	3.8
1	D	436	GLU	3.8
1	C	307	GLY	3.8
1	D	307	GLY	3.8
1	D	61	SER	3.8
1	E	123	ASN	3.7
1	C	427	LYS	3.7
1	E	252	GLN	3.7
1	C	32	GLU	3.7
1	F	366	ASP	3.7
1	D	417	PRO	3.7
1	D	402	SER	3.7
1	A	151	ASP	3.7
1	E	75	LEU	3.7
1	D	180	SER	3.6
1	E	303	ARG	3.6
1	D	190	TYR	3.6
1	E	157	ILE	3.6
1	E	62	VAL	3.6
1	C	391	TYR	3.6
1	E	326	ASN	3.6
1	E	27	PRO	3.6
1	E	151	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	282	ASN	3.6
1	D	209	THR	3.6
1	C	323	ALA	3.5
1	B	304	LYS	3.5
1	D	159	GLU	3.5
1	A	257	ALA	3.5
1	E	73	GLU	3.5
1	C	360	GLN	3.5
1	C	372	SER	3.5
1	E	235	LYS	3.5
1	C	366	ASP	3.5
1	A	141	GLU	3.5
1	D	114	ILE	3.5
1	B	132	VAL	3.5
1	E	436	GLU	3.5
1	D	422	SER	3.5
1	C	145	ILE	3.5
1	E	33	CYS	3.5
1	D	405	ILE	3.4
1	B	398	LYS	3.4
1	C	367	LYS	3.4
1	D	323	ALA	3.4
1	C	359	ARG	3.4
1	F	91	VAL	3.4
1	F	397	ASP	3.4
1	C	406	VAL	3.4
1	C	29	LEU	3.4
1	E	163	THR	3.4
1	E	137	GLU	3.3
1	E	272	ALA	3.3
1	B	153	ASP	3.3
1	E	246	ALA	3.3
1	E	256	ALA	3.3
1	D	227	ASN	3.3
1	E	162	VAL	3.3
1	E	125	ASN	3.3
1	E	273	ILE	3.3
1	F	140	SER	3.2
1	D	169	GLU	3.2
1	E	80	GLY	3.2
1	C	305	ASN	3.2
1	F	436	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	136	GLN	3.2
1	C	289	GLN	3.2
1	E	179	PRO	3.2
1	F	327	ASP	3.2
1	C	324	LYS	3.2
1	F	158	ASP	3.1
1	A	123	ASN	3.1
1	E	304	LYS	3.1
1	E	347	LEU	3.1
1	D	29	LEU	3.1
1	F	258	ARG	3.1
1	A	174	ASN	3.1
1	F	402	SER	3.1
1	F	154	ASP	3.1
1	C	308	LYS	3.1
1	E	140	SER	3.1
1	C	303	ARG	3.1
1	F	263	SER	3.1
1	B	225	VAL	3.1
1	E	247	GLY	3.1
1	C	325	ALA	3.1
1	C	144	GLU	3.1
1	B	327	ASP	3.0
1	E	302	LYS	3.0
1	F	78	LEU	3.0
1	E	14	TYR	3.0
1	D	183	THR	3.0
1	C	348	ASP	3.0
1	D	401	GLU	3.0
1	F	172	ASP	3.0
1	B	305	ASN	3.0
1	D	134	PRO	3.0
1	D	258	ARG	3.0
1	C	209	THR	3.0
1	C	250	ASN	3.0
1	C	261	PHE	3.0
1	A	376	GLU	3.0
1	F	264	GLU	3.0
1	C	53	GLN	3.0
1	C	292	ASN	3.0
1	E	169	GLU	3.0
1	E	122	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	348	ASP	3.0
1	D	305	ASN	2.9
1	D	253	LYS	2.9
1	A	159	GLU	2.9
1	E	227	ASN	2.9
1	C	304	LYS	2.9
1	D	322	PRO	2.9
1	B	144	GLU	2.9
1	C	349	VAL	2.9
1	C	94	THR	2.9
1	A	263	SER	2.9
1	C	310	VAL	2.9
1	D	140	SER	2.9
1	D	414	ARG	2.9
1	E	173	GLY	2.9
1	A	172	ASP	2.9
1	D	368	ARG	2.9
1	E	310	VAL	2.9
1	D	222	ASN	2.9
1	D	60	GLN	2.9
1	C	399	GLU	2.8
1	D	48	ILE	2.8
1	C	205	SER	2.8
1	D	406	VAL	2.8
1	B	141	GLU	2.8
1	C	223	ASP	2.8
1	D	109	GLN	2.8
1	D	365	GLN	2.8
1	F	307	GLY	2.8
1	B	326	ASN	2.7
1	C	27	PRO	2.8
1	C	251	ALA	2.7
1	F	400	SER	2.7
1	D	27	PRO	2.7
1	E	170	SER	2.7
1	C	238	ASN	2.7
1	E	419	GLY	2.7
1	F	435	LEU	2.7
1	C	306	PRO	2.7
1	E	152	ASP	2.7
1	F	248	SER	2.7
1	F	94	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	136	GLN	2.7
1	E	30	ILE	2.7
1	E	434	ASN	2.7
1	C	125	ASN	2.7
1	B	151	ASP	2.7
1	D	26	GLU	2.7
1	F	401	GLU	2.7
1	C	77	GLN	2.7
1	D	118	GLN	2.7
1	E	12	ASN	2.7
1	E	404	ASN	2.7
1	D	144	GLU	2.7
1	C	158	ASP	2.7
1	C	285	ASP	2.7
1	C	275	GLU	2.7
1	E	175	ILE	2.7
1	C	122	GLU	2.6
1	C	436	GLU	2.6
1	E	233	MET	2.6
1	E	258	ARG	2.6
1	F	169	GLU	2.6
1	E	281	ILE	2.6
1	A	62	VAL	2.6
1	E	184	GLU	2.6
1	C	190	TYR	2.6
1	C	273	ILE	2.6
1	F	92	ALA	2.6
1	F	253	LYS	2.6
1	F	399	GLU	2.6
1	A	170	SER	2.6
1	A	348	ASP	2.6
1	C	315	ASP	2.6
1	C	422	SER	2.6
1	D	62	VAL	2.6
1	E	245	THR	2.6
1	C	208	LYS	2.6
1	B	90	SER	2.6
1	B	101	CYS	2.6
1	F	359	ARG	2.6
1	C	193	LYS	2.6
1	C	282	ASN	2.6
1	F	136	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	304	LYS	2.6
1	A	304	LYS	2.6
1	B	376	GLU	2.5
1	A	365	GLN	2.5
1	E	255	LYS	2.5
1	C	368	ARG	2.5
1	C	394	ASP	2.5
1	E	224	ASP	2.5
1	D	255	LYS	2.5
1	D	398	LYS	2.5
1	E	22	SER	2.5
1	E	269	LEU	2.5
1	F	393	ASP	2.5
1	E	234	GLY	2.5
1	F	183	THR	2.5
1	E	222	ASN	2.5
1	C	56	ASP	2.5
1	C	364	ARG	2.5
1	F	422	SER	2.5
1	C	278	ASN	2.5
1	C	269	LEU	2.5
1	F	324	LYS	2.5
1	C	270	SER	2.5
1	D	299	ARG	2.5
1	E	274	GLY	2.5
1	F	45	HIS	2.5
1	E	301	THR	2.5
1	E	257	ALA	2.5
1	D	72	GLY	2.5
1	D	176	THR	2.5
1	E	58	LYS	2.5
1	E	76	PRO	2.5
1	C	79	GLY	2.5
1	D	264	GLU	2.5
1	E	168	ILE	2.5
1	C	435	LEU	2.5
1	E	15	ALA	2.5
1	D	22	SER	2.4
1	B	223	ASP	2.4
1	F	171	ALA	2.4
1	B	375	ARG	2.4
1	E	74	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	276	ILE	2.4
1	E	431	ASN	2.4
1	C	34	PRO	2.4
1	D	364	ARG	2.4
1	C	405	ILE	2.4
1	D	392	ARG	2.4
1	E	156	SER	2.4
1	D	247	GLY	2.4
1	B	415	ASP	2.4
1	E	399	GLU	2.4
1	B	365	GLN	2.4
1	A	265	ASP	2.4
1	F	433	VAL	2.4
1	A	122	GLU	2.4
1	C	300	GLN	2.4
1	F	261	PHE	2.4
1	F	62	VAL	2.4
1	A	254	ILE	2.4
1	E	31	LYS	2.4
1	F	29	LEU	2.4
1	D	133	LYS	2.4
1	B	363	GLN	2.3
1	C	291	VAL	2.3
1	C	12	ASN	2.3
1	A	307	GLY	2.3
1	E	63	ASP	2.3
1	A	326	ASN	2.3
1	E	241	ARG	2.3
1	C	420	THR	2.3
1	E	110	LYS	2.3
1	C	265	ASP	2.3
1	C	309	ARG	2.3
1	A	358	SER	2.3
1	D	132	VAL	2.3
1	E	279	SER	2.3
1	C	262	ALA	2.3
1	B	266	TRP	2.3
1	C	28	GLU	2.3
1	F	165	TYR	2.3
1	D	175	ILE	2.3
1	D	413	HIS	2.3
1	C	415	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	136	GLN	2.3
1	D	397	ASP	2.3
1	C	342	LYS	2.3
1	F	377	SER	2.3
1	D	182	PHE	2.3
1	F	141	GLU	2.3
1	F	20	LEU	2.2
1	D	415	ASP	2.2
1	D	433	VAL	2.2
1	E	167	GLU	2.2
1	E	428	GLU	2.2
1	D	145	ILE	2.2
1	C	74	LYS	2.2
1	F	150	THR	2.2
1	B	377	SER	2.2
1	F	262	ALA	2.2
1	F	396	TYR	2.2
1	B	260	ASP	2.2
1	D	51	THR	2.2
1	D	232	GLU	2.2
1	E	116	ILE	2.2
1	A	303	ARG	2.2
1	B	292	ASN	2.2
1	E	194	ARG	2.2
1	C	54	ASP	2.2
1	C	385	ASP	2.2
1	E	379	GLN	2.2
1	F	153	ASP	2.2
1	D	256	ALA	2.2
1	D	287	ALA	2.2
1	C	392	ARG	2.2
1	D	400	SER	2.2
1	B	431	ASN	2.2
1	C	281	ILE	2.2
1	B	224	ASP	2.2
1	E	265	ASP	2.2
1	F	144	GLU	2.2
1	E	331	ASN	2.2
1	E	261	PHE	2.2
1	D	266	TRP	2.2
1	E	135	ILE	2.2
1	C	301	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	327	ASP	2.2
1	D	193	LYS	2.2
1	C	429	TYR	2.2
1	D	18	ALA	2.2
1	C	255	LYS	2.2
1	D	96	THR	2.2
1	B	121	ILE	2.2
1	C	135	ILE	2.2
1	F	161	LEU	2.2
1	C	140	SER	2.2
1	F	117	ALA	2.2
1	D	259	ARG	2.1
1	D	375	ARG	2.1
1	D	290	SER	2.1
1	F	356	GLN	2.1
1	E	66	SER	2.1
1	C	184	GLU	2.1
1	D	327	ASP	2.1
1	B	93	SER	2.1
1	C	167	GLU	2.1
1	C	219	MET	2.1
1	D	357	LEU	2.1
1	C	246	ALA	2.1
1	C	159	GLU	2.1
1	F	195	ARG	2.1
1	C	295	TRP	2.1
1	C	343	MET	2.1
1	F	110	LYS	2.1
1	E	60	GLN	2.1
1	C	62	VAL	2.1
1	C	196	ASN	2.1
1	A	264	GLU	2.1
1	D	309	ARG	2.1
1	B	255	LYS	2.1
1	C	254	ILE	2.1
1	F	357	LEU	2.1
1	D	106	GLU	2.1
1	F	270	SER	2.1
1	E	92	ALA	2.1
1	C	414	ARG	2.1
1	E	244	VAL	2.1
1	B	434	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	180	SER	2.1
1	B	118	GLN	2.1
1	C	434	ASN	2.1
1	F	395	TYR	2.1
1	B	25	THR	2.0
1	C	247	GLY	2.0
1	D	313	MET	2.0
1	A	153	ASP	2.0
1	A	258	ARG	2.0
1	C	227	ASN	2.0
1	C	264	GLU	2.0
1	D	376	GLU	2.0
1	C	150	THR	2.0
1	D	230	SER	2.0
1	E	190	TYR	2.0
1	F	18	ALA	2.0
1	C	78	LEU	2.0
1	A	399	GLU	2.0
1	B	436	GLU	2.0
1	F	152	ASP	2.0
1	A	235	LYS	2.0
1	D	160	ALA	2.0
1	E	262	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.