



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 AM UTC

PDB ID : 3BGW / pdb_00003bgw
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

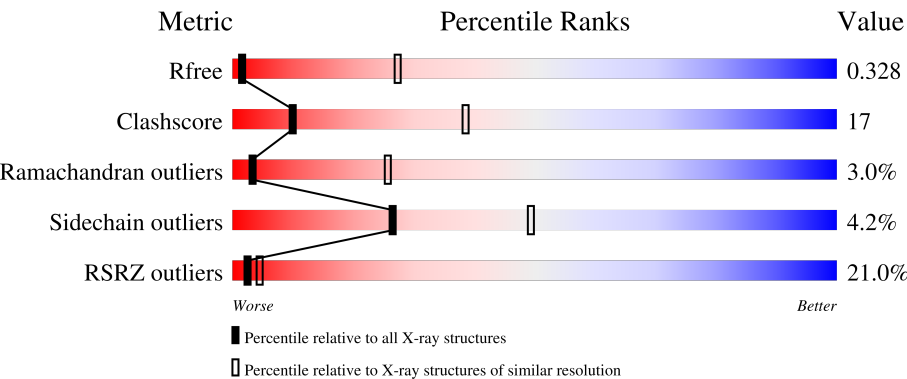
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)

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

Mol	Chain	Length	Quality of chain
1	A	444	18% 61%28%••6%
1	B	444	17% 65%25%••6%
1	C	444	23% 65%25%•6%
1	D	444	21% 65%23%•8%
1	E	444	23% 66%24%•6%

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Mol	Chain	Length	Quality of chain
1	F	444	17% 64% 25% • • 6%

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			

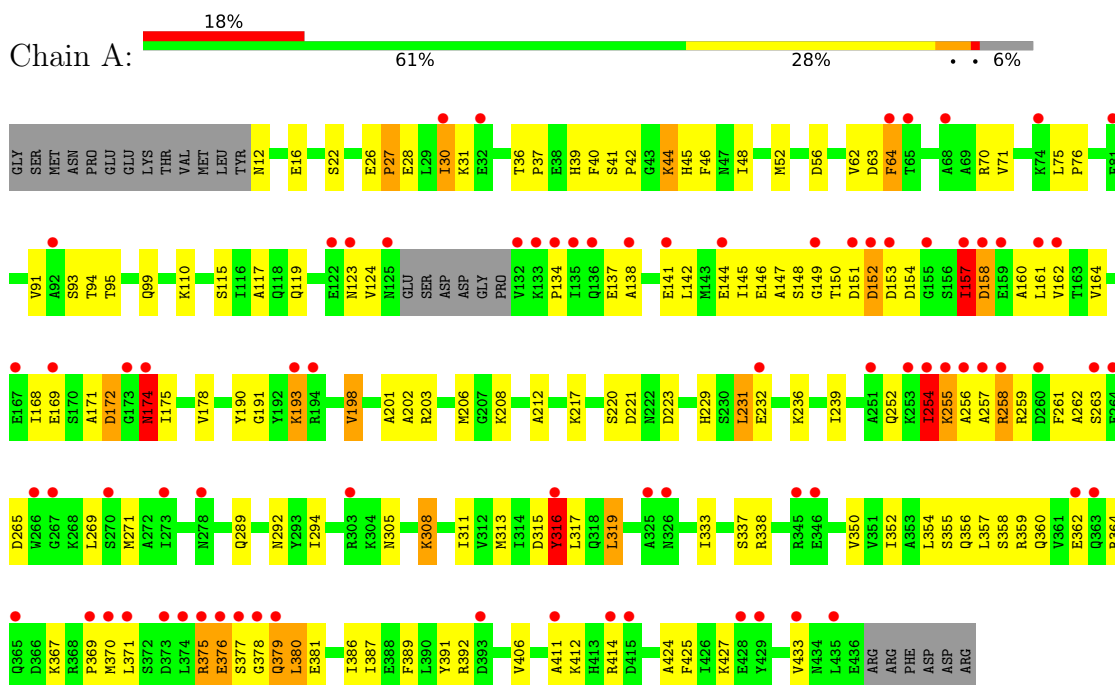
There are 12 discrepancies between the modelled and reference sequences:

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

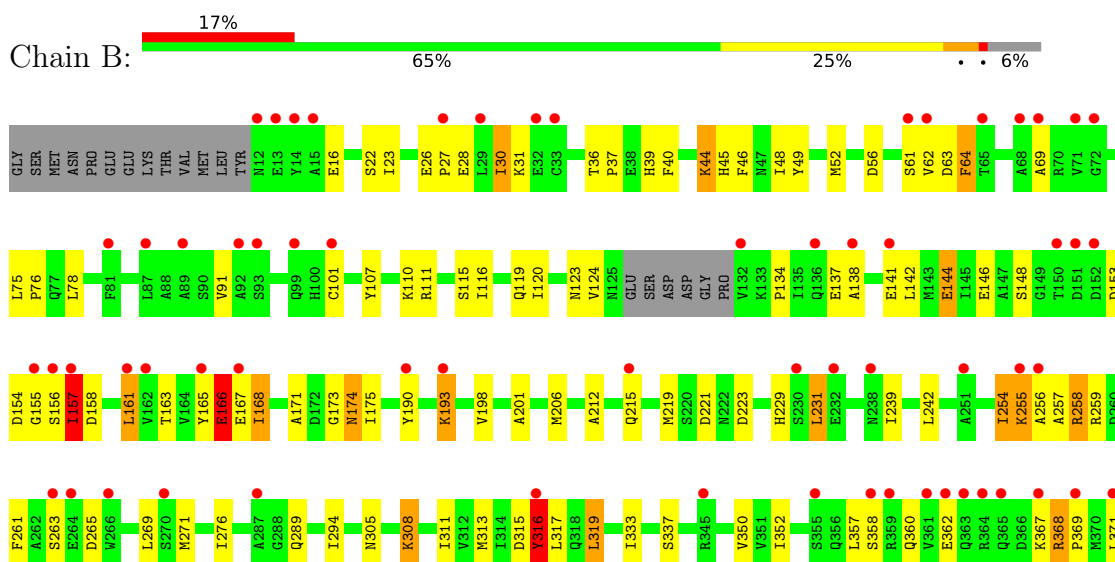
3 Residue-property plots [i](#)

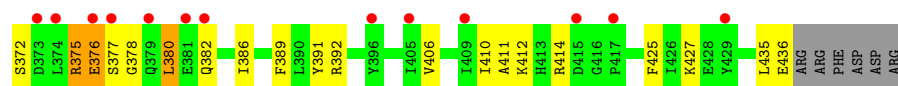
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNAB-Like Replicative Helicase

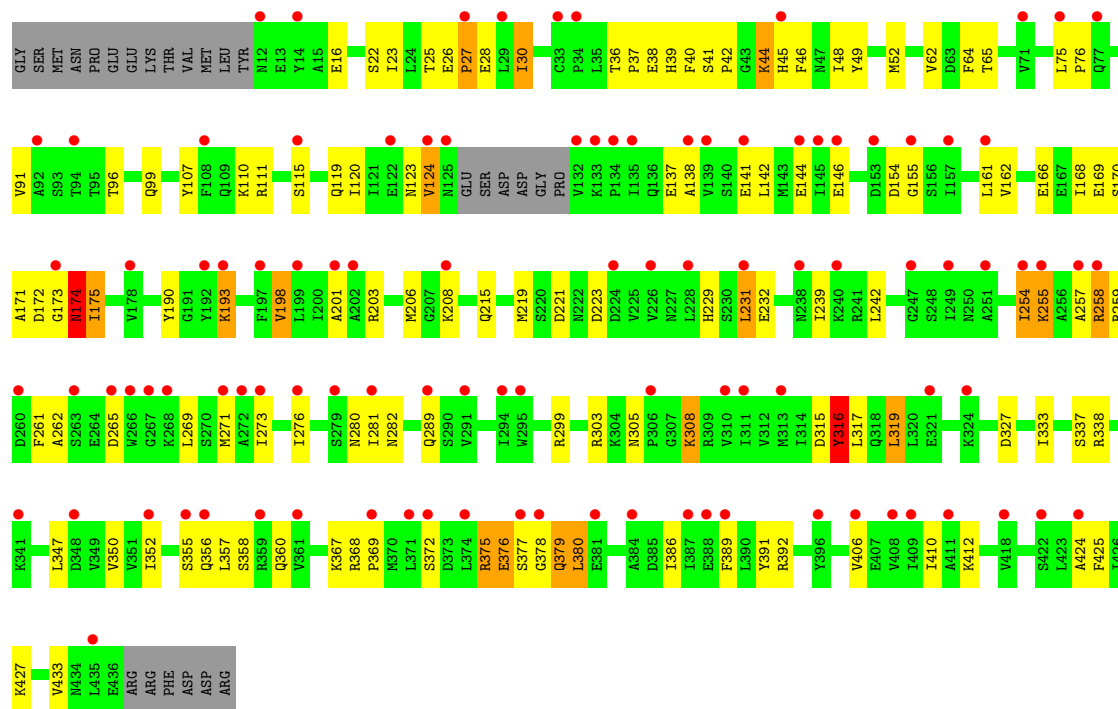


• Molecule 1: DNAB-Like Replicative Helicase

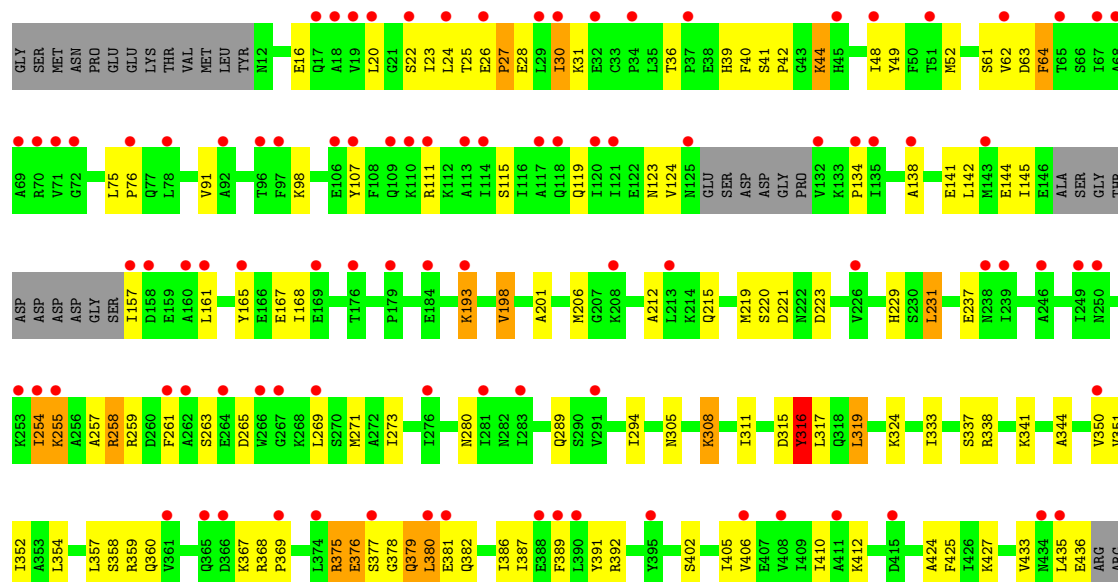




● Molecule 1: DNAB-Like Replicative Helicase



● Molecule 1: DNAB-Like Replicative Helicase



ASP
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.63Å 184.41Å 184.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 3.91 38.81 – 3.91	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.81-3.91) 97.3 (38.81-3.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 152.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	19724	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.39	2/3345 (0.1%)	0.73	0/4507
1	B	0.33	0/3345	0.71	3/4507 (0.1%)
1	C	0.37	3/3345 (0.1%)	0.72	1/4507 (0.0%)
1	D	0.34	0/3280	0.72	0/4417
1	E	0.39	2/3345 (0.1%)	0.73	1/4507 (0.0%)
1	F	0.46	5/3345 (0.1%)	0.76	4/4507 (0.1%)
All	All	0.38	12/20005 (0.1%)	0.73	9/26952 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	174	ASN	CA-C	-10.75	1.39	1.52
1	E	173	GLY	C-O	-10.67	1.10	1.23
1	F	174	ASN	C-O	-8.68	1.13	1.23
1	F	174	ASN	CA-CB	-8.43	1.39	1.53
1	F	174	ASN	CB-CG	-7.73	1.32	1.52
1	C	174	ASN	CG-OD1	-6.20	1.11	1.23
1	A	174	ASN	CB-CG	-6.10	1.36	1.52
1	A	174	ASN	CA-CB	-6.07	1.44	1.53
1	C	174	ASN	CB-CG	-5.99	1.37	1.52
1	E	173	GLY	N-CA	5.44	1.50	1.45
1	C	174	ASN	N-CA	-5.26	1.40	1.46
1	F	174	ASN	N-CA	-5.00	1.39	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	174	ASN	N-CA-C	12.16	127.39	108.79
1	E	173	GLY	O-C-N	-8.14	114.83	123.45
1	F	174	ASN	CA-CB-CG	-7.05	105.55	112.60
1	C	174	ASN	N-CA-CB	-5.90	101.70	110.90
1	F	174	ASN	N-CA-CB	-5.81	102.55	111.56
1	B	168	ILE	N-CA-C	-5.35	106.58	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	368	ARG	CA-C-N	5.24	125.00	119.76
1	B	368	ARG	C-N-CA	5.24	125.00	119.76
1	F	160	ALA	N-CA-C	-5.13	107.02	113.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	151	0
1	B	3298	0	3279	130	0
1	C	3298	0	3279	129	0
1	D	3234	0	3234	116	0
1	E	3298	0	3279	126	0
1	F	3298	0	3277	139	0
All	All	19724	0	19627	686	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 17.

All (686) 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:A:174:ASN:N	1:A:174:ASN:OD1	1.63	1.05
1:F:52:MET:HG3	1:F:62:VAL:HG11	1.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:239:ILE:HD13	1:F:161:LEU:HG	1.46	0.94
1:A:157:ILE:HG23	1:A:158:ASP:H	1.29	0.94
1:E:377:SER:HB2	1:E:380:LEU:HB2	1.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ASN:OD1	1:B:174:ASN:N	2.17	0.78
1:A:317:LEU:HD21	1:A:380:LEU:HD21	1.66	0.77
1:F:157:ILE:HG13	1:F:158:ASP:N	1.99	0.77
1:E:157:ILE:HG13	1:E:158:ASP:N	1.95	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
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:H	1:C:175:ILE:HD12	1.51	0.73
1:E:232:GLU:CD	1:F:414:ARG:HD3	2.11	0.73
1:E:168:ILE:CG1	1:E:169:GLU:H	1.95	0.73
1:D:75:LEU:N	1:D:76:PRO:HD2	2.03	0.73
1:F:52:MET:HG3	1:F:62:VAL:CG1	2.18	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:B:193:LYS:O	1:B:350:VAL:HG22	1.89	0.72
1:F:75:LEU:N	1:F:76:PRO:HD2	2.05	0.72
1:F:158:ASP:OD1	1:F:161:LEU:HD13	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:D:107:TYR:O	1:D:111:ARG:HG3	1.90	0.72
1:E:392:ARG:HG3	1:E:406:VAL:HG22	1.71	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:HD12	1:B:231:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:206:MET:HE3	1:F:391:TYR:HA	1.75	0.69
1:A:231:LEU:H	1:A:231:LEU:HD12	1.58	0.68
1:F:107:TYR:O	1:F:111:ARG:HG3	1.93	0.68
1:E:239:ILE:HD11	1:F:161:LEU:HG	1.76	0.68
1:A:26:GLU:O	1:A:28:GLU:N	2.26	0.68
1:B:124:VAL:HG11	1:C:110:LYS:HG3	1.74	0.68
1:D:124:VAL:CG1	1:E:110:LYS:HG3	2.23	0.68
1:B:362:GLU:HB2	1:C:372:SER:HB3	1.76	0.68
1:C:206:MET:HE3	1:C:391:TYR:HA	1.76	0.67
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:C:119:GLN:HG3	1:C:123:ASN:ND2	2.10	0.67
1:D:392:ARG:HG3	1:D:406:VAL:HG22	1.74	0.67
1:A:157:ILE:CG2	1:A:158:ASP:H	2.07	0.67
1:E:231:LEU:HD12	1:E:231:LEU:H	1.60	0.67
1:F:315:ASP:O	1:F:316:TYR:CB	2.41	0.67
1:C:356:GLN:HE22	1:D:379:GLN:CD	2.02	0.66
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:174:ASN:O	1:C:175:ILE:C	2.39	0.66
1:B:206:MET:HE3	1:B:391:TYR:HA	1.77	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:E:206:MET:HE3	1:E:391:TYR:HA	1.78	0.65
1:A:206:MET:HE3	1:A:391:TYR:HA	1.79	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:A:124:VAL:HG11	1:F:110:LYS:HG3	1.79	0.65
1:D:52:MET:CG	1:D:62:VAL:HG11	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ILE:O	1:E:52:MET:HB2	1.96	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:A:26:GLU:C	1:A:28:GLU:H	2.04	0.64
1:A:36:THR:H	1:A:39:HIS:CD2	2.14	0.64
1:E:273:ILE:HG23	1:F:165:TYR:HE2	1.60	0.64
1:E:315:ASP:O	1:E:316:TYR:CB	2.41	0.64
1:F:392:ARG:HG3	1:F:406:VAL:HG22	1.79	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:257:ALA:HB1	1:F:261:PHE:CB	2.27	0.64
1:F:377:SER:HB2	1:F:380:LEU: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
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:C:356:GLN:CD	1:D:382:GLN:OE1	2.42	0.63
1:A:315:ASP:O	1:A:316:TYR:CB	2.40	0.62
1:B:175:ILE:HD12	1:B:175:ILE:H	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:A:154:ASP:HB3	1:F:300:GLN:HE22	1.65	0.61
1:D:333:ILE:HG21	1:D:377:SER:HB3	1.82	0.61
1:D:206:MET:HE3	1:D:391:TYR:HA	1.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:THR:H	1:D:39:HIS:CD2	2.18	0.60
1:F:378:GLY:C	1:F:380:LEU:H	2.09	0.60
1:D:231:LEU:HD12	1:D:231:LEU:H	1.65	0.60
1:C:107:TYR:O	1:C:111:ARG:HG3	2.01	0.60
1:D:257:ALA:HB1	1:D:261:PHE:CB	2.31	0.60
1:B:259:ARG:H	1:C:171:ALA:HB3	1.66	0.60
1:C:203:ARG:NH2	1:D:381:GLU:OE1	2.32	0.60
1:C:317:LEU:CD2	1:C:380:LEU:HD21	2.29	0.60
1:E:158:ASP:C	1:E:160:ALA:H	2.08	0.60
1:E:255:LYS:HG2	1:F:190:TYR:CD1	2.37	0.60
1:F:254:ILE:O	1:F:255:LYS:C	2.44	0.60
1:A:124:VAL:HG13	1:A:134:PRO:HB3	1.83	0.59
1:A:157:ILE:CG2	1:A:158:ASP:N	2.65	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:A:254:ILE:O	1:A:255:LYS:C	2.46	0.59
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:C:48:ILE:O	1:C:52:MET:HB2	2.03	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: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:B:333:ILE:HG21	1:B:377:SER:HB3	1.84	0.58
1:C:172:ASP:C	1:C:174:ASN:H	2.09	0.58
1:D:98:LYS:HE2	1:D:98:LYS:HA	1.84	0.58
1:E:317:LEU:CD2	1:E:380:LEU:HD21	2.32	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:378:GLY:C	1:C:380:LEU:H	2.12	0.58
1:B:156:SER:C	1:B:157:ILE:HG13	2.29	0.57
1:C:257:ALA:HB1	1:C:261:PHE:CB	2.34	0.57
1:F:212:ALA:HB1	1:F:313:MET:HE1	1.85	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:A:378:GLY:C	1:A:380:LEU:H	2.11	0.57
1:C:254:ILE:HA	1:C:258:ARG:HB2	1.86	0.57
1:D:254:ILE:O	1:D:255:LYS:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:GLY:C	1:D:380:LEU:H	2.12	0.57
1:B:305:ASN:HB3	1:B:308:LYS:HD2	1.85	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:A:316:TYR:HB3	1:A:319:LEU:HB2	1.87	0.57
1:B:165:TYR:O	1:B:166:GLU:C	2.47	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:16:GLU:OE2	1:C:40:PHE:HA	2.05	0.57
1:C:316:TYR:HB3	1:C:319:LEU:HB2	1.87	0.57
1:D:22:SER:N	1:D:91:VAL:HG21	2.19	0.57
1:D:316:TYR:HB3	1:D:319:LEU:HB2	1.87	0.57
1:A:258:ARG:CG	1:B:168:ILE:HG23	2.32	0.57
1:B:37:PRO:HB2	1:B:46:PHE:CE1	2.39	0.57
1:E:254:ILE:HA	1:E:258:ARG:HB2	1.85	0.57
1:B:254:ILE:O	1:B:255:LYS:C	2.48	0.56
1:B:124:VAL:CG1	1:C:110:LYS:HG3	2.35	0.56
1:D:48:ILE:O	1:D:52:MET:HB2	2.04	0.56
1:F:375:ARG:HE	1:F:376:GLU:HG3	1.70	0.56
1:A:93:SER:C	1:A:95:THR:H	2.14	0.56
1:A:236:LYS:NZ	1:B:163:THR:HG21	2.20	0.56
1:B:375:ARG:HE	1:B:376:GLU:HG3	1.71	0.56
1:C:254:ILE:O	1:C:255:LYS:C	2.48	0.56
1:D:305:ASN:HB3	1:D:308:LYS:HD2	1.88	0.56
1:C:22:SER:N	1:C:91:VAL:HG21	2.20	0.56
1:F:254:ILE:HG23	1:F:255:LYS:H	1.71	0.56
1:A:254:ILE:HG13	1:B:168:ILE:CD1	2.34	0.56
1:A:254:ILE:HA	1:A:258:ARG:HB2	1.88	0.56
1:C:299:ARG:HB3	1:C:299:ARG:NH1	2.20	0.56
1:E:119:GLN:HG3	1:E:123:ASN:ND2	2.20	0.56
1:E:254:ILE:O	1:E:255:LYS:C	2.49	0.56
1:B:26:GLU:C	1:B:28:GLU:H	2.14	0.56
1:C:299:ARG:NH1	1:D:31:LYS:O	2.39	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:F:220:SER:HG	1:F:280:ASN:H	1.54	0.55
1:B:157:ILE:O	1:B:161:LEU:N	2.34	0.55
1:B:212:ALA:HB1	1:B:313:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:378:GLY:C	1:B:380:LEU:H	2.14	0.55
1:A:146:GLU:C	1:A:148:SER:H	2.14	0.55
1:B:257:ALA:HB1	1:B:261:PHE:CB	2.36	0.55
1:C:282:ASN:HA	1:D:157:ILE:HG23	1.89	0.55
1:B:254:ILE:HA	1:B:258:ARG:HB2	1.89	0.55
1:D:317:LEU:CD2	1:D:380:LEU:HD21	2.35	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:A:212:ALA:HB1	1:A:313:MET:HE1	1.89	0.54
1:B:317:LEU:CD2	1:B:380:LEU:HD21	2.35	0.54
1:A:375:ARG:HE	1:A:376:GLU:HG3	1.72	0.54
1:A:392:ARG:HH21	1:A:427:LYS:HE2	1.73	0.54
1:D:254:ILE:HG23	1:D:255:LYS:H	1.73	0.54
1:B:165:TYR:O	1:B:168:ILE:HG12	2.08	0.54
1:D:315:ASP:O	1:D:316:TYR:CB	2.42	0.54
1:E:99:GLN:HE22	1:F:61:SER:H	1.54	0.54
1:E:378:GLY:C	1:E:380:LEU:H	2.14	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:B:229:HIS:CD2	1:B:294:ILE:HG12	2.43	0.54
1:F:48:ILE:O	1:F:52:MET:HB2	2.08	0.54
1:D:201:ALA:O	1:D:389:PHE:HA	2.07	0.54
1:E:162:VAL:O	1:E:165:TYR:HB2	2.08	0.53
1:E:424:ALA:HB3	1:E:433:VAL:HB	1.90	0.53
1:C:52:MET:CG	1:C:62:VAL:HG11	2.28	0.53
1:D:23:ILE:HG21	1:D:30:ILE:HG23	1.89	0.53
1:B:357:LEU:HD13	1:B:369:PRO:HB3	1.90	0.53
1:C:392:ARG:HH21	1:C:427:LYS:HE2	1.72	0.53
1:A:138:ALA:O	1:A:142:LEU:HB2	2.08	0.53
1:C:96:THR:HG22	1:D:61:SER:OG	2.09	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:F:316:TYR:HD2	1:F:319:LEU:HD13	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:257:ALA:HB1	1:A:261:PHE:CB	2.39	0.53
1:D:161:LEU:HD23	1:D:161:LEU:O	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: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:A:356:GLN:HE22	1:B:382:GLN:CD	2.17	0.52
1:E:282:ASN:HA	1:F:157:ILE:HB	1.89	0.52
1:A:99:GLN:HE22	1:B:61:SER:H	1.57	0.52
1:F:52:MET:CG	1:F:62:VAL:HG11	2.24	0.52
1:C:115:SER:O	1:C:119:GLN:HB2	2.09	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:D:26:GLU:C	1:D:28:GLU:H	2.17	0.52
1:A:160:ALA:O	1:A:164:VAL:HG23	2.10	0.52
1:B:201:ALA:O	1:B:389:PHE:HA	2.10	0.52
1:B:259:ARG:NH1	1:C:169:GLU:HG2	2.24	0.52
1:D:157:ILE:HG13	1:D:157:ILE:O	2.09	0.52
1:E:392:ARG:HH21	1:E:427:LYS:HE2	1.74	0.52
1:F:123:ASN:HB3	1:F:137:GLU:OE1	2.09	0.52
1:A:362:GLU:HB2	1:B:372:SER:HB3	1.91	0.52
1:C:26:GLU:C	1:C:28:GLU:H	2.18	0.52
1:C:41:SER:HB3	1:C:42:PRO:HD2	1.91	0.52
1:F:392:ARG:HH21	1:F:427:LYS:HE2	1.73	0.52
1:C:232:GLU:HG3	1:D:341:LYS:HE2	1.91	0.52
1:E:115:SER:O	1:E:119:GLN:HB2	2.09	0.52
1:F:16:GLU:OE2	1:F:40:PHE:HA	2.10	0.52
1:A:269:LEU:C	1:A:271:MET:H	2.17	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:316:TYR:HD2	1:E:319:LEU:HD13	1.75	0.51
1:B:64:PHE:CD1	1:B:64:PHE:N	2.78	0.51
1:A:305:ASN:HB3	1:A:308:LYS:HD2	1.93	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ILE:HA	1:D:258:ARG:HB2	1.93	0.51
1:B:254:ILE:HG23	1:B:255:LYS:H	1.76	0.51
1:C:356:GLN:OE1	1:D:382:GLN:OE1	2.29	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:169:GLU:HB2	1:F:259:ARG:NH1	2.26	0.50
1:A:316:TYR:HD2	1:A:319:LEU:HD13	1.76	0.50
1:D:16:GLU:OE2	1:D:40:PHE:HA	2.11	0.50
1:D:75:LEU:N	1:D:76:PRO:CD	2.73	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:A:371:LEU:HD11	1:A:411:ALA:HB1	1.94	0.50
1:B:435:LEU:O	1:B:436:GLU:HB2	2.11	0.50
1:E:375:ARG:HE	1:E:376:GLU:HG3	1.75	0.50
1:A:175:ILE:HD12	1:A:175:ILE:N	2.26	0.50
1:E:208:LYS:HD2	1:E:355:SER:O	2.11	0.50
1:E:254:ILE:HD11	1:F:168:ILE:HD12	1.94	0.50
1:B:110:LYS:HG3	1:C:124:VAL:CG1	2.41	0.50
1:A:115:SER:O	1:A:119:GLN:HB2	2.11	0.50
1:A:256:ALA:O	1:B:171:ALA:HB1	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
1:C:424:ALA:HB3	1:C:433:VAL:HB	1.93	0.50
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:B:137:GLU:O	1:B:141:GLU:HG2	2.13	0.49
1:D:358:SER:HB2	1:D:375:ARG:HB2	1.94	0.49
1:D:435:LEU:O	1:D:436:GLU:C	2.55	0.49
1:E:26:GLU:C	1:E:28:GLU:H	2.20	0.49
1:C:303:ARG:NH1	1:D:98:LYS:HD2	2.27	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:198:VAL:HG22	1:C:352:ILE:HG12	1.94	0.49
1:F:257:ALA:O	1:F:258:ARG:C	2.55	0.49
1:D:157:ILE:O	1:D:157:ILE:CG1	2.59	0.49
1:F:138:ALA:O	1:F:142:LEU:HB2	2.13	0.49
1:D:237:GLU:CD	1:E:415:ASP:HA	2.37	0.49
1:E:167:GLU:HA	1:E:170:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:16:GLU:OE2	1:B:40:PHE:HA	2.12	0.48
1:F:41:SER:O	1:F:46:PHE:HB2	2.12	0.48
1:A:141:GLU:O	1:A:145:ILE:HG13	2.12	0.48
1:B:119:GLN:HG3	1:B:123:ASN:HD22	1.77	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:F:64:PHE:CD1	1:F:64:PHE:N	2.82	0.48
1:F:280:ASN:N	1:F:280:ASN:HD22	2.11	0.48
1:B:239:ILE:HG21	1:C:161:LEU:HG	1.96	0.48
1:D:338:ARG:HG3	1:D:379:GLN:HG2	1.95	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:F:146:GLU:C	1:F:148:SER:H	2.22	0.48
1:B:258:ARG:HB3	1:C:171:ALA:CB	2.44	0.48
1:E:232:GLU:CD	1:F:414:ARG:HH11	2.18	0.48
1:B:386:ILE:HA	1:B:412:LYS:O	2.14	0.48
1:E:142:LEU:O	1:E:146:GLU:HG3	2.14	0.48
1:E:337:SER:HB2	1:E:380:LEU:HD22	1.95	0.48
1:D:359:ARG:NH1	1:E:366:ASP:HB3	2.29	0.48
1:F:406:VAL:HG23	1:F:425:PHE:CB	2.42	0.48
1:B:362:GLU:HB2	1:C:372:SER:CB	2.41	0.48
1:F:125:ASN:OD1	1:F:125:ASN:N	2.46	0.48
1:F:337:SER:HB2	1:F:380:LEU:HD22	1.96	0.48
1:B:116:ILE:HG12	1:B:144:GLU:HB3	1.95	0.47
1:E:282:ASN:ND2	1:F:157:ILE:HD13	2.29	0.47
1:A:157:ILE:HD13	1:A:158:ASP:HA	1.96	0.47
1:C:142:LEU:O	1:C:146:GLU:HG3	2.14	0.47
1:A:414:ARG:O	1:F:237:GLU:OE1	2.32	0.47
1:E:239:ILE:HD11	1:F:161:LEU:CG	2.43	0.47
1:A:31:LYS:HE3	1:A:56:ASP:OD1	2.14	0.47
1:B:175:ILE:HD12	1:B:175:ILE:N	2.28	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: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:B:337:SER:HB2	1:B:380:LEU:HD22	1.95	0.47
1:D:220:SER:HG	1:D:280:ASN:H	1.62	0.47
1:F:257:ALA:O	1:F:259:ARG:N	2.48	0.47
1:E:316:TYR:CD2	1:E:319:LEU:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:SER:HB2	1:F:375:ARG:HB2	1.95	0.47
1:A:229:HIS:CD2	1:A:294:ILE:HG12	2.50	0.47
1:E:282:ASN:ND2	1:F:157:ILE:CD1	2.78	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:152:ASP:N	1:A:152:ASP:OD1	2.48	0.46
1:B:316:TYR:CD2	1:B:319:LEU:HD13	2.50	0.46
1:C:154:ASP:CG	1:C:155:GLY:N	2.72	0.46
1:A:142:LEU:O	1:A:146:GLU:HG3	2.14	0.46
1:A:171:ALA:O	1:A:172:ASP:C	2.59	0.46
1:B:138:ALA:O	1:B:142:LEU:HB2	2.15	0.46
1:E:160:ALA:O	1:E:164:VAL:N	2.42	0.46
1:C:201:ALA:O	1:C:389:PHE:HA	2.16	0.46
1:C:410:ILE:HD12	1:C:410:ILE:N	2.31	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:44:LYS:O	1:E:48:ILE:HG12	2.15	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:E:157:ILE:CG1	1:E:158:ASP:N	2.70	0.46
1:F:174:ASN:O	1:F:175:ILE:O	2.34	0.46
1:A:26:GLU:C	1:A:28:GLU:N	2.71	0.46
1:A:269:LEU:C	1:A:271:MET:N	2.74	0.46
1:A:217:LYS:O	1:A:220:SER:N	2.49	0.46
1:A:259:ARG:HB3	1:B:171:ALA:O	2.16	0.46
1:C:358:SER:C	1:C:360:GLN:H	2.24	0.46
1:F:254:ILE:O	1:F:258:ARG:HB2	2.16	0.46
1:F:316:TYR:CD2	1:F:319:LEU:HD13	2.50	0.46
1:A:64:PHE:CD1	1:A:64:PHE:N	2.84	0.46
1:C:41:SER:O	1:C:46:PHE:HB2	2.16	0.46
1:D:406:VAL:HG23	1:D:425:PHE:CB	2.45	0.46
1:E:362:GLU:HB2	1:F:372:SER:HB3	1.97	0.46
1:E:406:VAL:HG23	1:E:425:PHE:CB	2.45	0.46
1:A:239:ILE:HD13	1:B:161:LEU:HD22	1.97	0.46
1:D:221:ASP:C	1:D:223:ASP:H	2.24	0.46
1:A:358:SER:C	1:A:360:GLN:H	2.23	0.46
1:B:221:ASP:C	1:B:223:ASP:H	2.24	0.46
1:F:26:GLU:C	1:F:28:GLU:H	2.23	0.46
1:B:146:GLU:C	1:B:148:SER:H	2.23	0.45
1:E:137:GLU:O	1:E:141:GLU:HG2	2.16	0.45
1:E:368:ARG:HA	1:E:369:PRO:HD3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ASP:O	1:B:64:PHE:C	2.58	0.45
1:F:257:ALA:HB1	1:F:261:PHE:HB2	1.98	0.45
1:A:12:ASN:HD21	1:B:69:ALA:HA	1.81	0.45
1:E:229:HIS:CD2	1:E:294:ILE:HG12	2.52	0.45
1:A:158:ASP:C	1:A:160:ALA:N	2.74	0.45
1:B:258:ARG:HB3	1:C:171:ALA:HB2	1.97	0.45
1:C:254:ILE:HG23	1:C:255:LYS:H	1.81	0.45
1:C:269:LEU:C	1:C:271:MET:H	2.22	0.45
1:D:215:GLN:HB3	1:D:219:MET:HE3	1.99	0.45
1:F:269:LEU:C	1:F:271:MET:H	2.23	0.45
1:E:254:ILE:HG23	1:E:255:LYS:H	1.81	0.45
1:A:203:ARG:NH1	1:A:359:ARG:HA	2.31	0.45
1:C:208:LYS:HD2	1:C:355:SER:O	2.17	0.45
1:D:41:SER:HB3	1:D:42:PRO:HD2	1.98	0.45
1:B:175:ILE:H	1:B:175:ILE:CD1	2.29	0.45
1:B:406:VAL:HG23	1:B:425:PHE:CB	2.45	0.45
1:E:169:GLU:O	1:E:170:SER:O	2.35	0.45
1:E:172:ASP:OD2	1:E:172:ASP:N	2.50	0.45
1:E:381:GLU:HA	1:E:387:ILE:HD11	1.98	0.45
1:C:257:ALA:O	1:C:258:ARG:C	2.60	0.45
1:C:299:ARG:HB3	1:C:299:ARG:HH11	1.82	0.45
1:E:356:GLN:OE1	1:F:382:GLN:HG2	2.17	0.45
1:C:406:VAL:HG23	1:C:425:PHE:CB	2.45	0.45
1:E:158:ASP:C	1:E:160:ALA:N	2.68	0.45
1:E:175:ILE:N	1:E:175:ILE:HD12	2.31	0.45
1:E:254:ILE:O	1:E:258:ARG:HB2	2.16	0.45
1:F:254:ILE:HA	1:F:258:ARG:HD2	1.99	0.45
1:F:406:VAL:CG2	1:F:425:PHE:HB2	2.44	0.45
1:B:257:ALA:O	1:B:258:ARG:C	2.60	0.44
1:C:367:LYS:HB2	1:C:391:TYR:HE1	1.82	0.44
1:E:358:SER:C	1:E:360:GLN:H	2.24	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:E:232:GLU:CD	1:F:414:ARG:NH1	2.70	0.44
1:A:39:HIS:HE1	1:A:151:ASP:OD2	2.01	0.44
1:A:152:ASP:HB2	1:A:153:ASP:H	1.52	0.44
1:A:236:LYS:HZ1	1:B:163:THR:HG21	1.82	0.44
1:A:357:LEU:CD1	1:A:369:PRO:HB3	2.46	0.44
1:D:386:ILE:HA	1:D:412:LYS:O	2.18	0.44
1:E:220:SER:HG	1:E:280:ASN:H	1.66	0.44
1:A:316:TYR:CD2	1:A:319:LEU:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ASP:C	1:C:174:ASN:N	2.72	0.44
1:D:257:ALA:O	1:D:258:ARG:C	2.60	0.44
1:E:280:ASN:N	1:E:280:ASN:HD22	2.14	0.44
1:F:201:ALA:O	1:F:202:ALA:HB2	2.17	0.44
1:B:258:ARG:HG2	1:C:168:ILE:O	2.16	0.44
1:B:371:LEU:HD11	1:B:411:ALA:HB1	2.00	0.44
1:C:37:PRO:HB2	1:C:46:PHE:CE1	2.52	0.44
1:D:44:LYS:O	1:D:48:ILE:HG12	2.17	0.44
1:D:368:ARG:HA	1:D:369:PRO:HD3	1.81	0.44
1:A:201:ALA:O	1:A:389:PHE:HA	2.17	0.44
1:A:212:ALA:HB2	1:A:354:LEU:HD11	2.00	0.44
1:A:337:SER:HB2	1:A:380:LEU:HD22	1.99	0.44
1:E:269:LEU:C	1:E:271:MET:H	2.25	0.44
1:E:282:ASN:HD21	1:F:157:ILE:HD13	1.82	0.44
1:F:44:LYS:O	1:F:48:ILE:HG12	2.18	0.44
1:F:410:ILE:N	1:F:410:ILE:HD12	2.33	0.44
1:C:215:GLN:HB3	1:C:219:MET:HE3	1.98	0.44
1:D:410:ILE:N	1:D:410:ILE:HD12	2.33	0.44
1:F:376:GLU:CD	1:F:377:SER:H	2.26	0.44
1:A:212:ALA:HB1	1:A:313:MET:CE	2.48	0.44
1:A:232:GLU:CD	1:B:414:ARG:HD3	2.43	0.44
1:B:269:LEU:C	1:B:271:MET:H	2.26	0.44
1:E:171:ALA:O	1:E:172:ASP:HB3	2.17	0.44
1:A:154:ASP:CB	1:F:300:GLN:HE22	2.30	0.43
1:C:280:ASN:N	1:C:280:ASN:HD22	2.16	0.43
1:D:124:VAL:HG13	1:D:134:PRO:HB3	2.00	0.43
1:D:269:LEU:C	1:D:271:MET:H	2.26	0.43
1:E:201:ALA:O	1:E:389:PHE:HA	2.17	0.43
1:F:201:ALA:O	1:F:389:PHE:HA	2.19	0.43
1:A:30:ILE:HD12	1:A:31:LYS:H	1.83	0.43
1:A:178:VAL:O	1:A:191:GLY:HA2	2.18	0.43
1:A:356:GLN:NE2	1:B:382:GLN:CD	2.76	0.43
1:A:406:VAL:CG2	1:A:425:PHE:HB2	2.47	0.43
1:F:161:LEU:O	1:F:161:LEU:HD23	2.18	0.43
1:F:279:SER:C	1:F:280:ASN:HD22	2.26	0.43
1:A:259:ARG:CB	1:B:171:ALA:O	2.67	0.43
1:B:258:ARG:O	1:B:259:ARG:C	2.61	0.43
1:B:263:SER:C	1:B:265:ASP:H	2.26	0.43
1:C:254:ILE:HA	1:C:258:ARG:HD2	2.00	0.43
1:F:212:ALA:HB1	1:F:313:MET:CE	2.46	0.43
1:B:259:ARG:HB2	1:C:171:ALA:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ASP:O	1:D:64:PHE:C	2.61	0.43
1:E:257:ALA:O	1:E:258:ARG:C	2.61	0.43
1:A:406:VAL:HG23	1:A:425:PHE:CB	2.44	0.43
1:B:165:TYR:O	1:B:167:GLU:N	2.52	0.43
1:E:410:ILE:HD12	1:E:410:ILE:N	2.33	0.43
1:D:254:ILE:O	1:D:258:ARG:HB2	2.19	0.43
1:F:158:ASP:HA	1:F:161:LEU:HB3	2.00	0.43
1:B:358:SER:C	1:B:360:GLN:H	2.26	0.43
1:C:368:ARG:HA	1:C:369:PRO:HD3	1.79	0.43
1:D:311:ILE:HG13	1:D:350:VAL:HB	2.00	0.43
1:F:157:ILE:HG13	1:F:158:ASP:OD1	2.18	0.43
1:F:152:ASP:C	1:F:154:ASP:H	2.26	0.43
1:A:338:ARG:HG3	1:A:379:GLN:HG2	2.00	0.43
1:B:256:ALA:HB3	1:C:190:TYR:CE2	2.53	0.43
1:C:254:ILE:O	1:C:258:ARG:HB2	2.19	0.43
1:C:355:SER:OG	1:C:356:GLN:N	2.52	0.43
1:D:64:PHE:CD1	1:D:64:PHE:N	2.87	0.43
1:E:263:SER:C	1:E:265:ASP:H	2.27	0.43
1:A:63:ASP:O	1:A:64:PHE:C	2.62	0.42
1:B:215:GLN:HB3	1:B:219:MET:HE3	2.01	0.42
1:A:198:VAL:CG2	1:A:352:ILE:HG12	2.49	0.42
1:A:254:ILE:O	1:A:258:ARG:HB2	2.19	0.42
1:A:358:SER:HB2	1:A:375:ARG:HB2	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:257:ALA:O	1:A:258:ARG:C	2.62	0.42
1:A:263:SER:C	1:A:265:ASP:H	2.27	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:358:SER:C	1:D:360:GLN:H	2.27	0.42
1:D:254:ILE:HA	1:D:258:ARG:HD2	2.00	0.42
1:A:370:MET:HE1	1:F:359:ARG:HD3	2.01	0.42
1:B:367:LYS:HB2	1:B:391:TYR:HE1	1.85	0.42
1:D:402:SER:HB3	1:D:405:ILE:HB	2.02	0.42
1:E:119:GLN:HG3	1:E:123:ASN:HD22	1.84	0.42
1:E:367:LYS:HB2	1:E:391:TYR:HE1	1.85	0.42
1:F:119:GLN:HG3	1:F:123:ASN:HD22	1.84	0.42
1:A:208:LYS:HD2	1:A:355:SER:O	2.19	0.42
1:C:25:THR:O	1:C:27:PRO:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ILE:HD12	1:A:311:ILE:N	2.35	0.42
1:A:358:SER:C	1:A:360:GLN:N	2.77	0.42
1:E:358:SER:HB2	1:E:375:ARG:HB2	2.01	0.42
1:A:44:LYS:O	1:A:45:HIS:C	2.62	0.42
1:B:31:LYS:HE3	1:B:56:ASP:OD1	2.20	0.42
1:C:257:ALA:O	1:C:259:ARG:N	2.53	0.42
1:D:145:ILE:O	1:D:145:ILE:HG22	2.20	0.42
1:D:229:HIS:CD2	1:D:294:ILE:HG12	2.54	0.42
1:E:257:ALA:O	1:E:259:ARG:N	2.53	0.42
1:A:252:GLN:HG2	1:B:190:TYR:OH	2.19	0.42
1:D:378:GLY:C	1:D:380:LEU:N	2.77	0.42
1:E:163:THR:C	1:E:165:TYR:N	2.76	0.42
1:E:221:ASP:C	1:E:223:ASP:H	2.26	0.42
1:C:154:ASP:CG	1:C:155:GLY:H	2.28	0.41
1:C:242:LEU:HB3	1:C:276:ILE:HD12	2.01	0.41
1:F:31:LYS:HE3	1:F:56:ASP:OD1	2.20	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:A:381:GLU:HA	1:A:387:ILE:HD11	2.02	0.41
1:D:49:TYR:HA	1:D:52:MET:HB3	2.02	0.41
1:D:138:ALA:O	1:D:142:LEU:HB2	2.21	0.41
1:E:41:SER:O	1:E:46:PHE:HB2	2.20	0.41
1:F:148:SER:C	1:F:150:THR:H	2.28	0.41
1:B:44:LYS:O	1:B:45:HIS:C	2.62	0.41
1:C:258:ARG:O	1:C:259:ARG:C	2.64	0.41
1:C:386:ILE:HA	1:C:412:LYS:O	2.20	0.41
1:D:406:VAL:CG2	1:D:425:PHE:HB2	2.46	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:D:198:VAL:HG22	1:D:352:ILE:HG12	2.02	0.41
1:E:198:VAL:HG22	1:E:352:ILE:HG12	2.01	0.41
1:F:368:ARG:HA	1:F:369:PRO:HD3	1.79	0.41
1:A:160:ALA:O	1:A:161:LEU:C	2.64	0.41
1:A:311:ILE:HG13	1:A:350:VAL:HB	2.02	0.41
1:C:38:GLU:H	1:C:38:GLU:HG2	1.67	0.41
1:E:167:GLU:O	1:E:170:SER:HB2	2.20	0.41
1:F:26:GLU:HB2	1:F:29:LEU:HD22	2.02	0.41
1:A:117:ALA:C	1:A:119:GLN:H	2.28	0.41
1:A:150:THR:HG21	1:F:303:ARG:NH2	2.35	0.41
1:A:232:GLU:CD	1:B:414:ARG:NH1	2.75	0.41
1:B:166:GLU:C	1:B:168:ILE:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ALA:O	1:C:142:LEU:HB2	2.20	0.41
1:D:25:THR:O	1:D:27:PRO:HD3	2.21	0.41
1:F:163:THR:O	1:F:167:GLU:OE1	2.39	0.41
1:A:262:ALA:HB1	1:A:265:ASP:OD2	2.19	0.41
1:C:49:TYR:HA	1:C:52:MET:HB3	2.03	0.41
1:E:259:ARG:HB2	1:F:171:ALA:O	2.21	0.41
1:A:221:ASP:C	1:A:223:ASP:H	2.28	0.41
1:A:378:GLY:C	1:A:380:LEU:N	2.75	0.41
1:C:44:LYS:O	1:C:45:HIS:C	2.64	0.41
1:E:201:ALA:O	1:E:202:ALA:HB2	2.20	0.41
1:E:358:SER:C	1:E:360:GLN:N	2.79	0.41
1:F:262:ALA:HB1	1:F:265:ASP:OD2	2.20	0.41
1:F:381:GLU:HA	1:F:387:ILE:HD11	2.02	0.41
1:A:12:ASN:O	1:A:16:GLU:HB2	2.21	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:215:GLN:O	1:B:219:MET:HG3	2.20	0.41
1:B:242:LEU:HB3	1:B:276:ILE:HD12	2.03	0.41
1:B:311:ILE:N	1:B:311:ILE:HD12	2.36	0.41
1:B:410:ILE:HD12	1:B:410:ILE:N	2.36	0.41
1:E:124:VAL:HG13	1:E:134:PRO:HB3	2.02	0.41
1:E:326:ASN:HD22	1:E:326:ASN:HA	1.67	0.41
1:F:311:ILE:HD12	1:F:311:ILE:N	2.36	0.41
1:A:201:ALA:O	1:A:202:ALA:HB2	2.20	0.41
1:A:308:LYS:NZ	1:A:308:LYS:HB3	2.36	0.41
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:C:327:ASP:O	1:D:324:LYS:NZ	2.54	0.41
1:C:338:ARG:HG3	1:C:379:GLN:HG2	2.02	0.41
1:D:263:SER:C	1:D:265:ASP:H	2.29	0.41
1:D:344:ALA:HB2	1:D:351:VAL:CG2	2.51	0.41
1:E:38:GLU:H	1:E:38:GLU:HG2	1.65	0.41
1:E:313:MET:HA	1:E:352:ILE:O	2.21	0.41
1:F:212:ALA:HB2	1:F:354:LEU:HD11	2.02	0.41
1:A:367:LYS:HB2	1:A:391:TYR:HE1	1.86	0.40
1:C:269:LEU:C	1:C:271:MET:N	2.80	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:E:378:GLY:C	1:E:380:LEU:N	2.79	0.40
1:F:257:ALA:HB1	1:F:261:PHE:HB3	2.02	0.40
1:F:269:LEU:C	1:F:271:MET:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:313:MET:HA	1:B:352:ILE:O	2.21	0.40
1:D:337:SER:HB2	1:D:380:LEU:HD22	2.03	0.40
1:C:273:ILE:HD13	1:D:165:TYR:CD2	2.57	0.40
1:F:49:TYR:HA	1:F:52:MET:HB3	2.02	0.40
1:F:174:ASN:O	1:F:175:ILE:C	2.62	0.40
1:C:347:LEU:HD12	1:C:347:LEU:HA	1.89	0.40
1:D:212:ALA:HB2	1:D:354:LEU:HD11	2.04	0.40
1:E:254:ILE:HA	1:E:258:ARG:HD2	2.03	0.40
1:F:244:VAL:O	1:F:244:VAL:HG12	2.20	0.40
1:F:299:ARG:HB3	1:F:299:ARG:NH1	2.37	0.40
1:A:30:ILE:HD12	1:A:31:LYS:N	2.36	0.40
1:B:26:GLU:O	1:B:28:GLU:N	2.50	0.40
1:C:221:ASP:C	1:C:223:ASP:H	2.29	0.40
1:C:282:ASN:HA	1:D:157:ILE:CG2	2.52	0.40
1:C:376:GLU:CD	1:C:377:SER:H	2.29	0.40
1:F:358:SER:C	1:F:360:GLN:H	2.27	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%)	2	23
1	B	415/444 (94%)	357 (86%)	47 (11%)	11 (3%)	4	27
1	C	415/444 (94%)	365 (88%)	38 (9%)	12 (3%)	3	26
1	D	403/444 (91%)	355 (88%)	40 (10%)	8 (2%)	6	32
1	E	415/444 (94%)	358 (86%)	43 (10%)	14 (3%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	415/444 (94%)	354 (85%)	46 (11%)	15 (4%)	2	23
All	All	2478/2664 (93%)	2148 (87%)	255 (10%)	75 (3%)	3	26

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
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

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Mol	Chain	Res	Type
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
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%)	344 (95%)	17 (5%)	23	47
1	B	361/386 (94%)	345 (96%)	16 (4%)	25	48
1	C	361/386 (94%)	346 (96%)	15 (4%)	26	49
1	D	354/386 (92%)	342 (97%)	12 (3%)	32	55
1	E	361/386 (94%)	346 (96%)	15 (4%)	26	49
1	F	361/386 (94%)	346 (96%)	15 (4%)	26	49
All	All	2159/2316 (93%)	2069 (96%)	90 (4%)	26	49

All (90) 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	144	GLU
1	A	152	ASP
1	A	157	ILE
1	A	158	ASP
1	A	162	VAL
1	A	174	ASN
1	A	198	VAL
1	A	231	LEU
1	A	254	ILE
1	A	308	LYS
1	A	316	TYR
1	A	319	LEU
1	A	376	GLU
1	A	380	LEU
1	B	30	ILE
1	B	64	PHE
1	B	101	CYS
1	B	144	GLU
1	B	157	ILE

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Mol	Chain	Res	Type
1	B	161	LEU
1	B	166	GLU
1	B	174	ASN
1	B	198	VAL
1	B	231	LEU
1	B	254	ILE
1	B	308	LYS
1	B	316	TYR
1	B	319	LEU
1	B	376	GLU
1	B	380	LEU
1	C	30	ILE
1	C	64	PHE
1	C	65	THR
1	C	144	GLU
1	C	162	VAL
1	C	166	GLU
1	C	174	ASN
1	C	198	VAL
1	C	231	LEU
1	C	254	ILE
1	C	308	LYS
1	C	316	TYR
1	C	319	LEU
1	C	376	GLU
1	C	380	LEU
1	D	30	ILE
1	D	64	PHE
1	D	144	GLU
1	D	167	GLU
1	D	198	VAL
1	D	231	LEU
1	D	254	ILE
1	D	308	LYS
1	D	316	TYR
1	D	319	LEU
1	D	376	GLU
1	D	380	LEU
1	E	30	ILE
1	E	64	PHE
1	E	144	GLU
1	E	159	GLU

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Mol	Chain	Res	Type
1	E	165	TYR
1	E	167	GLU
1	E	174	ASN
1	E	198	VAL
1	E	231	LEU
1	E	254	ILE
1	E	308	LYS
1	E	316	TYR
1	E	319	LEU
1	E	376	GLU
1	E	380	LEU
1	F	30	ILE
1	F	64	PHE
1	F	125	ASN
1	F	144	GLU
1	F	150	THR
1	F	157	ILE
1	F	174	ASN
1	F	198	VAL
1	F	231	LEU
1	F	254	ILE
1	F	308	LYS
1	F	316	TYR
1	F	319	LEU
1	F	376	GLU
1	F	380	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) 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	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	60	GLN
1	B	77	GLN
1	B	99	GLN
1	B	100	HIS
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	99	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	229	HIS
1	C	280	ASN

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Mol	Chain	Res	Type
1	C	282	ASN
1	C	305	ASN
1	C	326	ASN
1	C	331	ASN
1	C	356	GLN
1	C	365	GLN
1	C	382	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	404	ASN
1	E	39	HIS
1	E	77	GLN
1	E	99	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

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Mol	Chain	Res	Type
1	E	305	ASN
1	E	326	ASN
1	E	331	ASN
1	E	356	GLN
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	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	419/444 (94%)	1.32	78 (18%) 3 6	103, 118, 142, 151	0
1	B	419/444 (94%)	1.26	76 (18%) 3 6	103, 117, 142, 151	0
1	C	419/444 (94%)	1.47	102 (24%) 2 4	103, 117, 142, 150	0
1	D	409/444 (92%)	1.48	95 (23%) 2 4	103, 117, 142, 150	0
1	E	419/444 (94%)	1.50	102 (24%) 2 4	103, 117, 142, 150	0
1	F	419/444 (94%)	1.38	74 (17%) 4 6	103, 117, 142, 151	0
All	All	2504/2664 (93%)	1.40	527 (21%) 2 4	103, 117, 142, 151	0

All (527) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	281	ILE	6.4
1	A	255	LYS	6.2
1	B	377	SER	6.0
1	C	279	SER	5.6
1	D	48	ILE	5.4
1	D	157	ILE	5.1
1	E	141	GLU	5.1
1	D	158	ASP	5.0
1	E	134	PRO	4.9
1	C	135	ILE	4.8
1	A	376	GLU	4.7
1	D	281	ILE	4.7
1	E	125	ASN	4.7
1	F	256	ALA	4.7
1	E	133	LYS	4.5
1	D	68	ALA	4.5
1	A	151	ASP	4.5
1	E	162	VAL	4.5
1	F	377	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	135	ILE	4.3
1	E	32	GLU	4.3
1	C	133	LYS	4.3
1	A	141	GLU	4.3
1	D	32	GLU	4.3
1	E	390	LEU	4.2
1	F	160	ALA	4.2
1	C	374	LEU	4.2
1	B	165	TYR	4.2
1	F	165	TYR	4.2
1	C	238	ASN	4.2
1	D	113	ALA	4.1
1	D	18	ALA	4.1
1	A	251	ALA	4.1
1	A	133	LYS	4.0
1	F	251	ALA	4.0
1	B	363	GLN	4.0
1	F	273	ILE	4.0
1	F	253	LYS	4.0
1	A	123	ASN	4.0
1	A	254	ILE	3.9
1	B	101	CYS	3.9
1	B	287	ALA	3.9
1	B	151	ASP	3.9
1	B	141	GLU	3.9
1	C	251	ALA	3.9
1	A	81	PHE	3.9
1	F	254	ILE	3.8
1	A	256	ALA	3.8
1	E	255	LYS	3.8
1	C	132	VAL	3.7
1	D	369	PRO	3.7
1	B	152	ASP	3.7
1	D	17	GLN	3.7
1	E	421	VAL	3.7
1	B	232	GLU	3.7
1	C	276	ILE	3.6
1	F	307	GLY	3.6
1	C	260	ASP	3.6
1	F	257	ALA	3.6
1	F	303	ARG	3.6
1	F	144	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	68	ALA	3.6
1	E	408	VAL	3.6
1	F	258	ARG	3.6
1	B	255	LYS	3.6
1	E	261	PHE	3.6
1	B	72	GLY	3.6
1	E	138	ALA	3.5
1	D	114	ILE	3.5
1	D	250	ASN	3.5
1	E	124	VAL	3.5
1	E	252	GLN	3.5
1	E	374	LEU	3.5
1	C	267	GLY	3.5
1	E	168	ILE	3.5
1	A	278	ASN	3.4
1	A	264	GLU	3.4
1	A	157	ILE	3.4
1	C	272	ALA	3.4
1	B	361	VAL	3.4
1	D	30	ILE	3.4
1	A	138	ALA	3.4
1	A	158	ASP	3.4
1	E	389	PHE	3.4
1	F	299	ARG	3.4
1	E	388	GLU	3.3
1	E	361	VAL	3.3
1	F	164	VAL	3.3
1	A	270	SER	3.3
1	E	362	GLU	3.3
1	C	255	LYS	3.3
1	C	134	PRO	3.3
1	D	71	VAL	3.3
1	D	261	PHE	3.3
1	D	22	SER	3.3
1	D	435	LEU	3.3
1	D	179	PRO	3.3
1	B	376	GLU	3.3
1	F	232	GLU	3.3
1	F	356	GLN	3.3
1	A	92	ALA	3.2
1	B	155	GLY	3.2
1	E	256	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	76	PRO	3.2
1	C	266	TRP	3.2
1	C	352	ILE	3.2
1	D	283	ILE	3.2
1	A	159	GLU	3.2
1	A	132	VAL	3.2
1	D	160	ALA	3.2
1	E	132	VAL	3.2
1	C	371	LEU	3.2
1	A	267	GLY	3.2
1	E	72	GLY	3.2
1	C	409	ILE	3.2
1	F	162	VAL	3.2
1	F	306	PRO	3.2
1	E	121	ILE	3.1
1	A	266	TRP	3.1
1	B	92	ALA	3.1
1	C	294	ILE	3.1
1	E	71	VAL	3.1
1	F	159	GLU	3.1
1	D	253	LYS	3.1
1	F	252	GLN	3.1
1	B	32	GLU	3.1
1	A	260	ASP	3.1
1	D	366	ASP	3.1
1	E	64	PHE	3.1
1	D	262	ALA	3.1
1	F	237	GLU	3.1
1	A	232	GLU	3.1
1	A	433	VAL	3.0
1	C	201	ALA	3.0
1	F	255	LYS	3.0
1	E	169	GLU	3.0
1	E	171	ALA	3.0
1	F	238	ASN	3.0
1	D	255	LYS	3.0
1	D	143	MET	3.0
1	E	369	PRO	3.0
1	A	173	GLY	3.0
1	E	246	ALA	3.0
1	D	121	ILE	3.0
1	F	161	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	69	ALA	3.0
1	A	273	ILE	2.9
1	C	193	LYS	2.9
1	D	110	LYS	2.9
1	F	261	PHE	2.9
1	A	373	ASP	2.9
1	D	395	TYR	2.9
1	E	113	ALA	2.9
1	D	269	LEU	2.9
1	C	271	MET	2.9
1	F	132	VAL	2.9
1	C	424	ALA	2.9
1	C	359	ARG	2.9
1	E	158	ASP	2.9
1	D	118	GLN	2.9
1	D	246	ALA	2.9
1	C	155	GLY	2.8
1	D	109	GLN	2.8
1	A	377	SER	2.8
1	A	135	ILE	2.8
1	E	373	ASP	2.8
1	B	396	TYR	2.8
1	E	232	GLU	2.8
1	C	92	ALA	2.8
1	E	359	ARG	2.8
1	F	345	ARG	2.8
1	D	29	LEU	2.8
1	D	67	ILE	2.8
1	B	238	ASN	2.8
1	B	68	ALA	2.8
1	E	254	ILE	2.7
1	F	277	SER	2.7
1	C	313	MET	2.7
1	B	362	GLU	2.7
1	C	141	GLU	2.7
1	D	276	ILE	2.7
1	D	291	VAL	2.7
1	F	267	GLY	2.7
1	D	51	THR	2.7
1	F	150	THR	2.7
1	A	415	ASP	2.7
1	C	295	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	365	GLN	2.7
1	D	24	LEU	2.7
1	D	374	LEU	2.7
1	A	65	THR	2.7
1	B	65	THR	2.7
1	E	51	THR	2.7
1	E	376	GLU	2.7
1	F	141	GLU	2.7
1	E	62	VAL	2.7
1	C	34	PRO	2.7
1	C	138	ALA	2.7
1	E	120	ILE	2.7
1	F	281	ILE	2.7
1	D	165	TYR	2.7
1	F	14	TYR	2.7
1	A	167	GLU	2.7
1	A	362	GLU	2.7
1	C	377	SER	2.7
1	E	350	VAL	2.6
1	A	303	ARG	2.6
1	F	283	ILE	2.6
1	E	208	LYS	2.6
1	F	434	ASN	2.6
1	B	81	PHE	2.6
1	E	79	GLY	2.6
1	F	316	TYR	2.6
1	E	146	GLU	2.6
1	B	156	SER	2.6
1	C	406	VAL	2.6
1	E	45	HIS	2.6
1	B	266	TRP	2.6
1	D	380	LEU	2.6
1	E	348	ASP	2.6
1	E	371	LEU	2.6
1	B	358	SER	2.6
1	D	434	ASN	2.6
1	B	132	VAL	2.6
1	A	258	ARG	2.6
1	C	254	ILE	2.6
1	D	135	ILE	2.6
1	F	135	ILE	2.6
1	B	367	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	77	GLN	2.6
1	B	264	GLU	2.6
1	A	379	GLN	2.6
1	E	89	ALA	2.6
1	D	176	THR	2.6
1	A	122	GLU	2.6
1	A	153	ASP	2.6
1	A	375	ARG	2.6
1	D	406	VAL	2.6
1	E	74	LYS	2.6
1	B	89	ALA	2.6
1	C	247	GLY	2.6
1	C	273	ILE	2.5
1	E	148	SER	2.5
1	C	231	LEU	2.5
1	D	390	LEU	2.5
1	C	411	ALA	2.5
1	D	267	GLY	2.5
1	B	157	ILE	2.5
1	B	190	TYR	2.5
1	C	361	VAL	2.5
1	B	138	ALA	2.5
1	C	139	VAL	2.5
1	E	139	VAL	2.5
1	F	151	ASP	2.5
1	E	157	ILE	2.5
1	B	14	TYR	2.5
1	B	61	SER	2.5
1	C	122	GLU	2.5
1	C	144	GLU	2.5
1	D	106	GLU	2.5
1	F	137	GLU	2.5
1	A	174	ASN	2.5
1	C	125	ASN	2.5
1	B	33	CYS	2.5
1	E	360	GLN	2.5
1	C	378	GLY	2.5
1	E	420	THR	2.5
1	A	370	MET	2.5
1	C	14	TYR	2.5
1	C	226	VAL	2.5
1	D	62	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	388	GLU	2.5
1	E	365	GLN	2.5
1	F	262	ALA	2.5
1	E	315	ASP	2.5
1	C	396	TYR	2.5
1	F	346	GLU	2.4
1	C	249	ILE	2.4
1	A	257	ALA	2.4
1	B	379	GLN	2.4
1	C	29	LEU	2.4
1	C	369	PRO	2.4
1	B	316	TYR	2.4
1	D	193	LYS	2.4
1	B	417	PRO	2.4
1	C	94	THR	2.4
1	F	418	VAL	2.4
1	D	97	PHE	2.4
1	E	145	ILE	2.4
1	E	396	TYR	2.4
1	B	374	LEU	2.4
1	C	161	LEU	2.4
1	D	365	GLN	2.4
1	A	64	PHE	2.4
1	A	162	VAL	2.4
1	D	361	VAL	2.4
1	D	381	GLU	2.4
1	E	411	ALA	2.4
1	B	263	SER	2.4
1	F	263	SER	2.4
1	D	65	THR	2.4
1	F	408	VAL	2.4
1	A	371	LEU	2.4
1	B	371	LEU	2.4
1	C	348	ASP	2.4
1	E	395	TYR	2.4
1	D	208	LYS	2.4
1	B	150	THR	2.4
1	A	161	LEU	2.4
1	B	162	VAL	2.4
1	E	48	ILE	2.4
1	F	94	THR	2.4
1	A	194	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	345	ARG	2.4
1	B	429	TYR	2.4
1	C	265	ASP	2.4
1	D	107	TYR	2.4
1	E	375	ARG	2.4
1	B	69	ALA	2.4
1	B	256	ALA	2.4
1	A	74	LYS	2.4
1	E	100	HIS	2.3
1	A	134	PRO	2.3
1	A	374	LEU	2.3
1	B	409	ILE	2.3
1	D	120	ILE	2.3
1	E	93	SER	2.3
1	D	19	VAL	2.3
1	E	406	VAL	2.3
1	B	359	ARG	2.3
1	A	429	TYR	2.3
1	D	213	LEU	2.3
1	F	422	SER	2.3
1	A	326	ASN	2.3
1	C	418	VAL	2.3
1	B	99	GLN	2.3
1	C	75	LEU	2.3
1	C	389	PHE	2.3
1	D	249	ILE	2.3
1	A	411	ALA	2.3
1	C	192	TYR	2.3
1	E	76	PRO	2.3
1	C	178	VAL	2.3
1	F	282	ASN	2.3
1	B	193	LYS	2.3
1	F	266	TRP	2.3
1	C	33	CYS	2.3
1	C	228	LEU	2.3
1	C	108	PHE	2.3
1	E	14	TYR	2.3
1	E	316	TYR	2.3
1	E	432	PHE	2.3
1	A	363	GLN	2.3
1	B	382	GLN	2.3
1	E	53	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	115	SER	2.3
1	C	422	SER	2.3
1	E	170	SER	2.3
1	B	62	VAL	2.3
1	E	310	VAL	2.3
1	C	45	HIS	2.3
1	F	259	ARG	2.3
1	A	435	LEU	2.3
1	E	357	LEU	2.3
1	D	389	PHE	2.3
1	E	114	ILE	2.3
1	C	77	GLN	2.3
1	F	363	GLN	2.3
1	A	263	SER	2.3
1	C	291	VAL	2.3
1	E	291	VAL	2.3
1	B	345	ARG	2.3
1	C	224	ASP	2.3
1	F	269	LEU	2.2
1	A	365	GLN	2.2
1	E	391	TYR	2.2
1	C	372	SER	2.2
1	B	27	PRO	2.2
1	B	364	ARG	2.2
1	E	394	ASP	2.2
1	C	12	ASN	2.2
1	D	238	ASN	2.2
1	D	117	ALA	2.2
1	C	268	LYS	2.2
1	F	304	LYS	2.2
1	B	13	GLU	2.2
1	F	169	GLU	2.2
1	A	369	PRO	2.2
1	E	430	GLY	2.2
1	C	387	ILE	2.2
1	D	254	ILE	2.2
1	E	409	ILE	2.2
1	B	15	ALA	2.2
1	B	87	LEU	2.2
1	E	84	LEU	2.2
1	E	142	LEU	2.2
1	B	167	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	71	VAL	2.2
1	F	134	PRO	2.2
1	C	145	ILE	2.2
1	A	152	ASP	2.2
1	D	125	ASN	2.2
1	C	324	LYS	2.2
1	D	138	ALA	2.2
1	F	147	ALA	2.2
1	F	323	ALA	2.2
1	F	136	GLN	2.2
1	B	29	LEU	2.2
1	B	230	SER	2.2
1	A	169	GLU	2.2
1	D	184	GLU	2.2
1	C	157	ILE	2.2
1	C	311	ILE	2.2
1	A	393	ASP	2.2
1	B	251	ALA	2.2
1	C	202	ALA	2.2
1	F	29	LEU	2.2
1	C	408	VAL	2.2
1	D	350	VAL	2.2
1	F	71	VAL	2.2
1	A	428	GLU	2.2
1	C	173	GLY	2.2
1	E	407	GLU	2.2
1	F	146	GLU	2.2
1	E	287	ALA	2.1
1	C	355	SER	2.1
1	F	194	ARG	2.1
1	A	316	TYR	2.1
1	F	225	VAL	2.1
1	A	155	GLY	2.1
1	C	197	PHE	2.1
1	C	146	GLU	2.1
1	C	306	PRO	2.1
1	F	302	LYS	2.1
1	E	201	ALA	2.1
1	B	215	GLN	2.1
1	C	289	GLN	2.1
1	B	415	ASP	2.1
1	B	71	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	266	TRP	2.1
1	C	208	LYS	2.1
1	C	341	LYS	2.1
1	D	34	PRO	2.1
1	D	169	GLU	2.1
1	F	179	PRO	2.1
1	F	378	GLY	2.1
1	D	92	ALA	2.1
1	D	111	ARG	2.1
1	D	411	ALA	2.1
1	E	238	ASN	2.1
1	B	270	SER	2.1
1	E	61	SER	2.1
1	A	30	ILE	2.1
1	C	356	GLN	2.1
1	E	281	ILE	2.1
1	C	310	VAL	2.1
1	A	378	GLY	2.1
1	B	369	PRO	2.1
1	E	322	PRO	2.1
1	A	32	GLU	2.1
1	C	381	GLU	2.1
1	D	20	LEU	2.1
1	F	68	ALA	2.1
1	B	93	SER	2.1
1	A	136	GLN	2.1
1	D	226	VAL	2.1
1	D	161	LEU	2.1
1	E	260	ASP	2.1
1	E	269	LEU	2.1
1	C	388	GLU	2.1
1	E	183	THR	2.1
1	A	414	ARG	2.1
1	C	258	ARG	2.1
1	A	253	LYS	2.1
1	C	257	ALA	2.1
1	C	384	ALA	2.1
1	C	263	SER	2.1
1	E	367	LYS	2.1
1	F	236	LYS	2.1
1	B	12	ASN	2.1
1	B	161	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	27	PRO	2.1
1	D	134	PRO	2.1
1	E	65	THR	2.1
1	D	239	ILE	2.1
1	F	276	ILE	2.1
1	A	325	ALA	2.1
1	E	68	ALA	2.1
1	E	215	GLN	2.1
1	E	326	ASN	2.1
1	C	435	LEU	2.1
1	D	78	LEU	2.1
1	D	132	VAL	2.1
1	E	423	LEU	2.1
1	F	62	VAL	2.1
1	B	373	ASP	2.0
1	B	381	GLU	2.0
1	D	26	GLU	2.0
1	D	70	ARG	2.0
1	D	415	ASP	2.0
1	B	355	SER	2.0
1	C	199	LEU	2.0
1	D	408	VAL	2.0
1	F	331	ASN	2.0
1	E	370	MET	2.0
1	D	72	GLY	2.0
1	A	193	LYS	2.0
1	C	240	LYS	2.0
1	A	346	GLU	2.0
1	D	264	GLU	2.0
1	F	38	GLU	2.0
1	D	377	SER	2.0
1	B	136	GLN	2.0
1	F	421	VAL	2.0
1	A	125	ASN	2.0
1	A	149	GLY	2.0
1	B	405	ILE	2.0
1	D	37	PRO	2.0
1	D	45	HIS	2.0
1	D	96	THR	2.0
1	A	144	GLU	2.0
1	C	321	GLU	2.0
1	C	153	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	81	PHE	2.0
1	E	184	GLU	2.0
1	F	63	ASP	2.0
1	C	124	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.