



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 08:53 PM EDT

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

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:

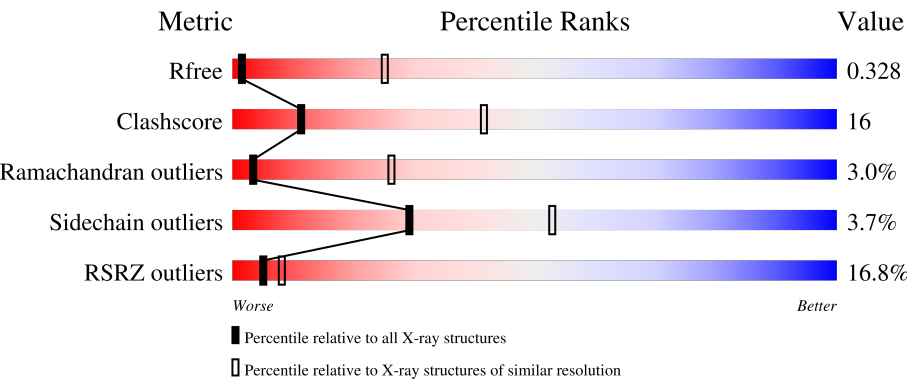
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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}	164625	1175 (4.14-3.70)
Clashscore	180529	1045 (4.12-3.72)
Ramachandran outliers	177936	1006 (4.12-3.72)
Sidechain outliers	177891	1185 (4.14-3.70)
RSRZ outliers	164620	1175 (4.14-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	<div><div>14%</div><div>63%</div><div>27%</div><div>• • 6%</div></div>
1	B	444	<div><div>15%</div><div>67%</div><div>23%</div><div>• • 6%</div></div>
1	C	444	<div><div>18%</div><div>67%</div><div>24%</div><div>• 6%</div></div>
1	D	444	<div><div>16%</div><div>68%</div><div>21%</div><div>• 8%</div></div>
1	E	444	<div><div>20%</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>13%</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			

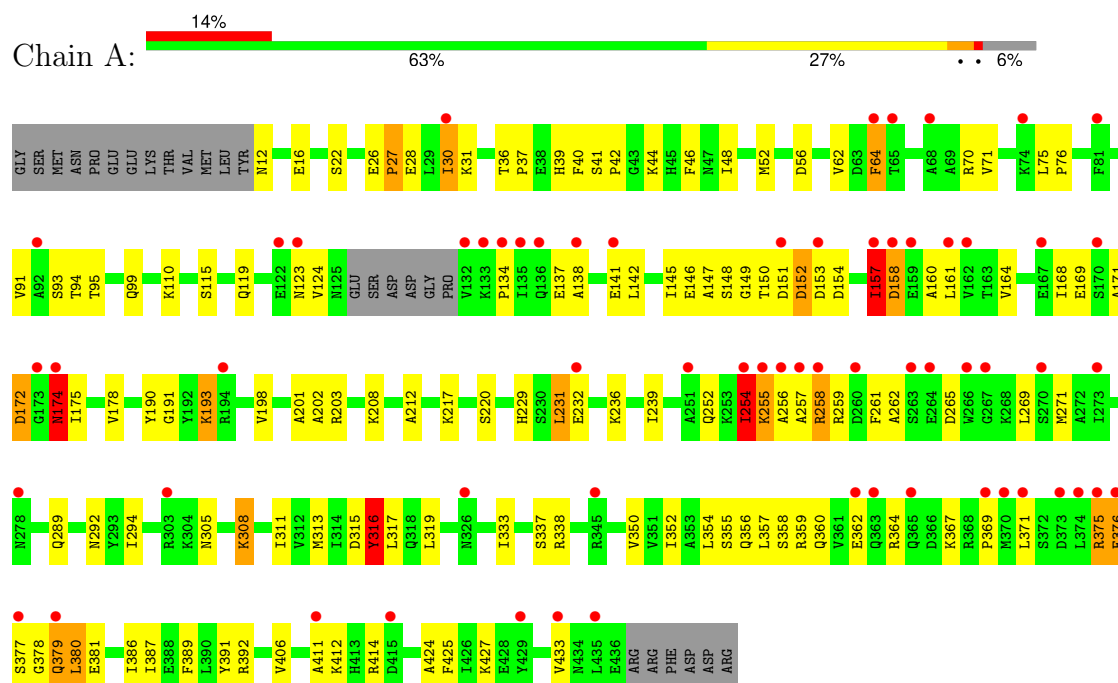
There are 12 discrepancies between the modelled and reference sequences:

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

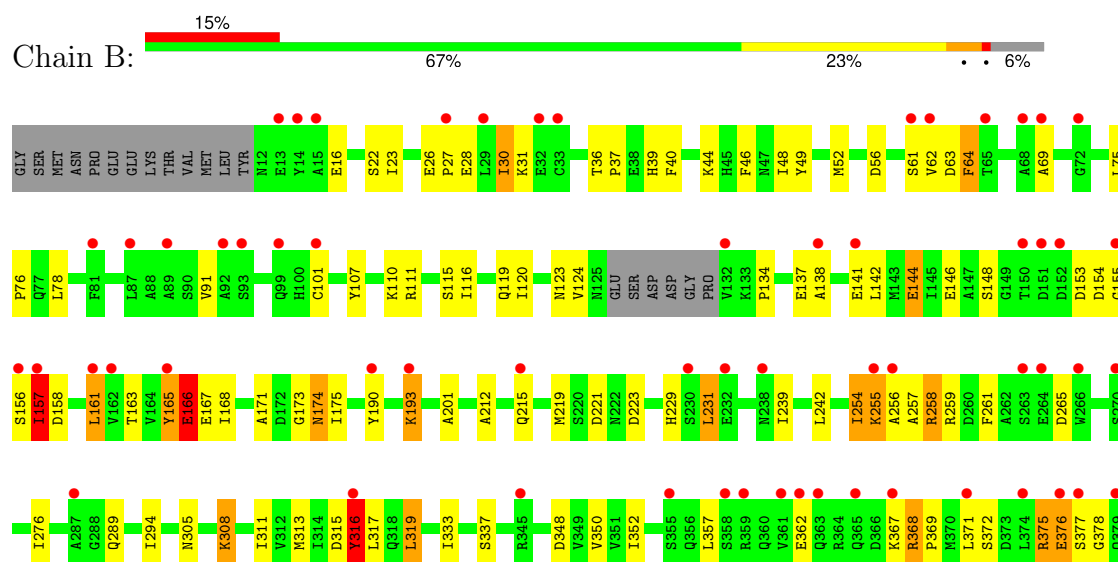
3 Residue-property plots [i](#)

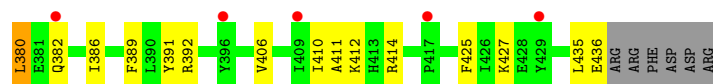
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

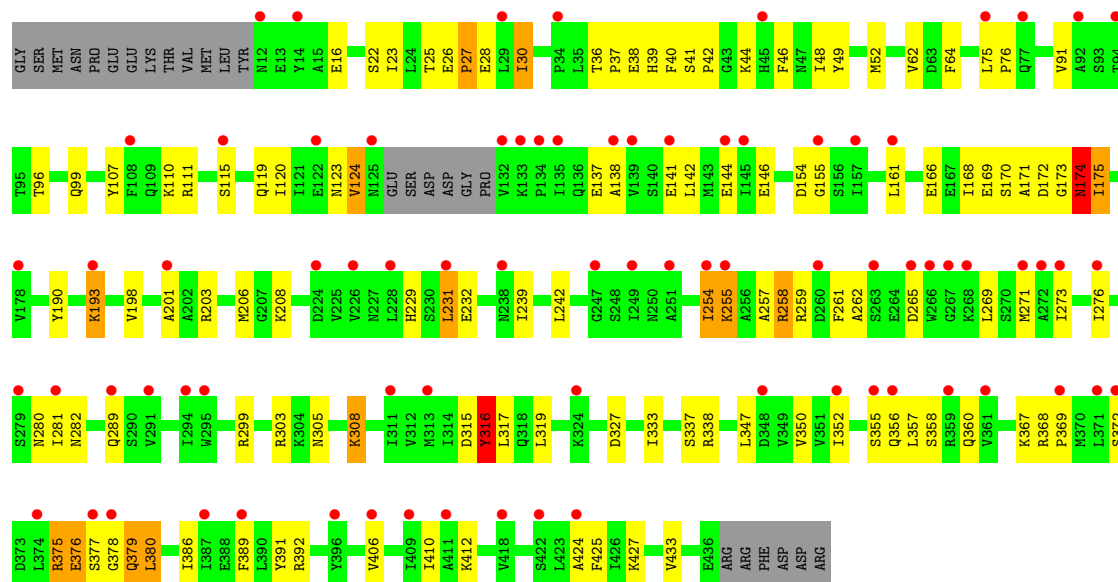


• Molecule 1: DNAB-Like Replicative Helicase

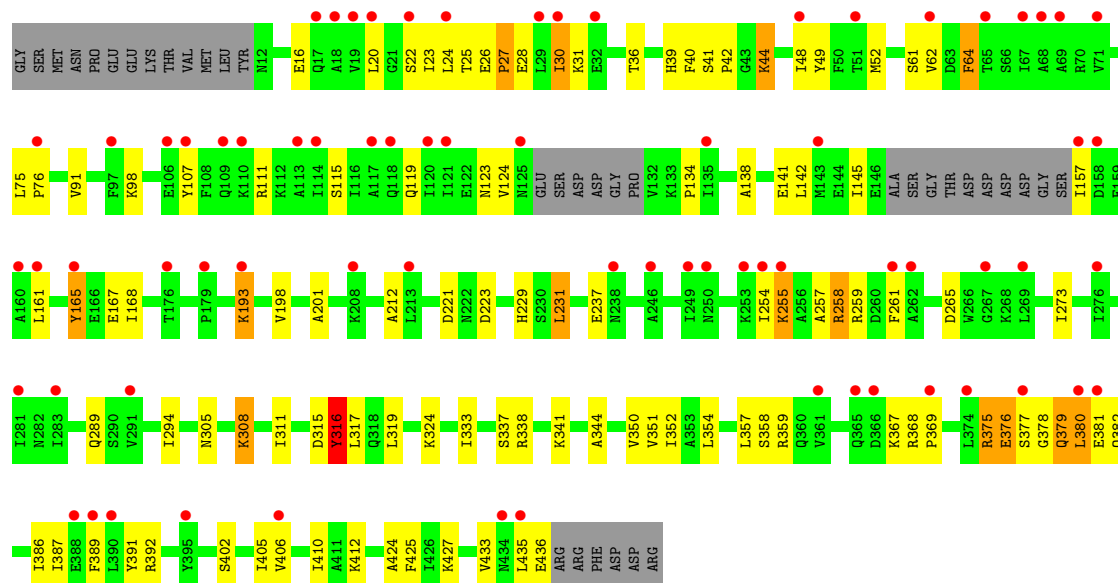




• Molecule 1: DNAB-Like Replicative Helicase

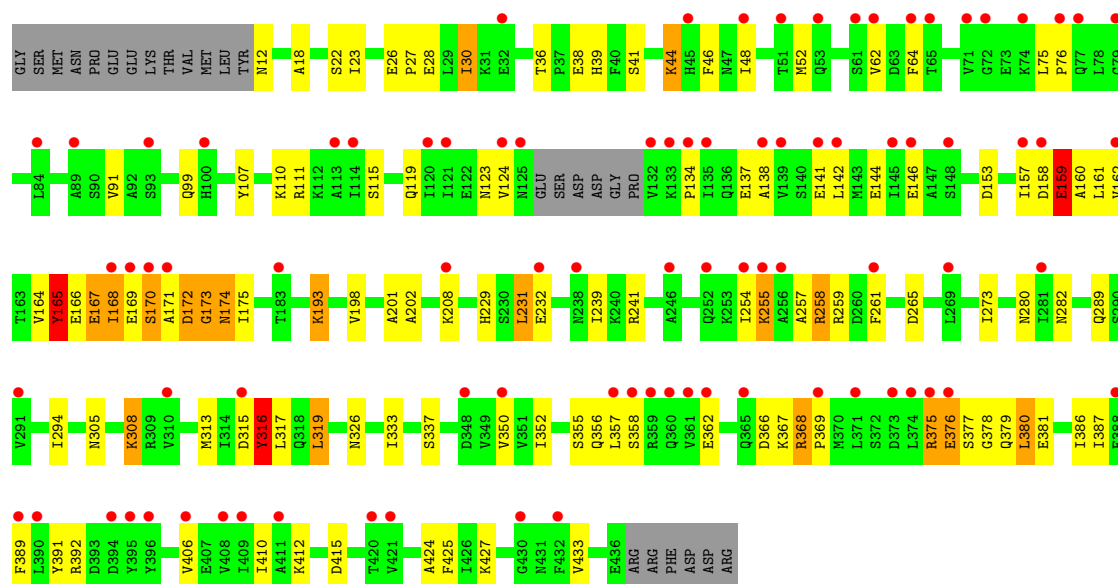


• Molecule 1: DNAB-Like Replicative Helicase

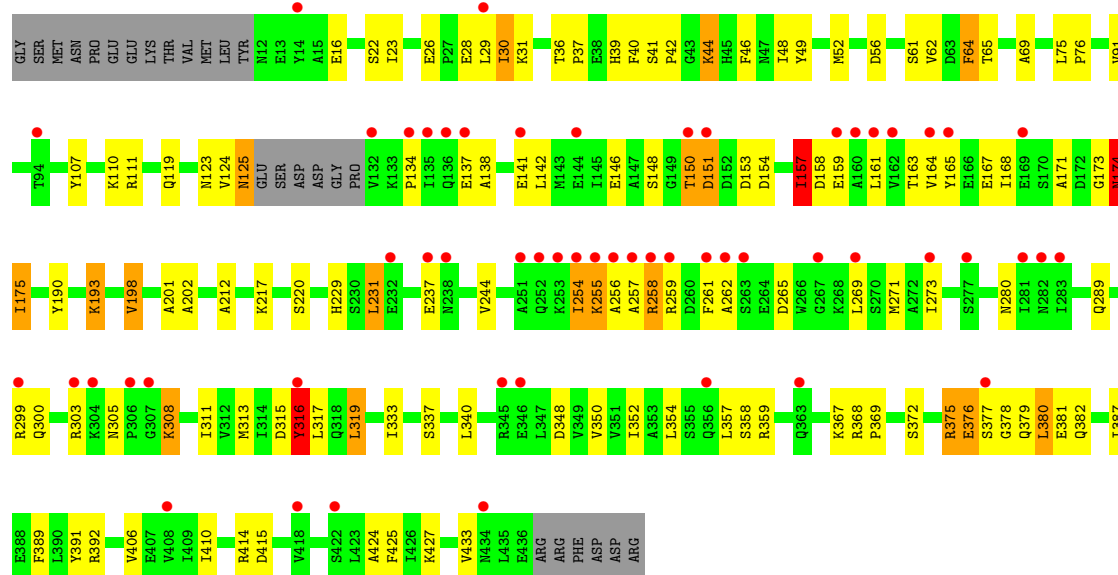


• Molecule 1: DNAB-Like Replicative Helicase





• 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, 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 (4.99%)	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	0.32	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($^{\circ}$)	Ideal($^{\circ}$)
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: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
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: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: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: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: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:H	1:C:175:ILE:HD12	1.51	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
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:E:232:GLU:CD	1:F:414:ARG:HD3	2.11	0.69
1:D:229:HIS:HD2	1:D:289:GLN:OE1	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

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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: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: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: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: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
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: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

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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: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:C:356:GLN:HE22	1:D:379:GLN:CD	2.02	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: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: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: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: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:164:VAL:O	1:A:168:ILE:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:356:GLN:CD	1:D:382:GLN:OE1	2.42	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: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: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: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: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: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: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

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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:B:157:ILE:O	1:B:161:LEU:N	2.34	0.55
1:E:158:ASP:C	1:E:160:ALA:H	2.08	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: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:F:254:ILE:O	1:F:255:LYS:C	2.44	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:254:ILE:O	1:A:255:LYS:C	2.46	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: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: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

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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: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
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:C:378:GLY:C	1:C:380:LEU:H	2.12	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: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:D:254:ILE:O	1:D:255:LYS:C	2.47	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:A:99:GLN:HE22	1:B:61:SER:H	1.57	0.52
1:B:165:TYR:O	1:B:166:GLU:C	2.47	0.52
1:F:52:MET:CG	1:F:62:VAL:HG11	2.24	0.52
1:B:156:SER:C	1:B:157:ILE:HG13	2.29	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: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:B:254:ILE:O	1:B:255:LYS:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:SER:C	1:A:95:THR:H	2.14	0.51
1:C:175:ILE:HD12	1:C:175:ILE:N	2.21	0.51
1:C:254:ILE:O	1:C:255:LYS:C	2.48	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:E:254:ILE:O	1:E:255:LYS:C	2.49	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: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
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:B:378:GLY:C	1:B:380:LEU:H	2.14	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:146:GLU:C	1:A:148:SER:H	2.14	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

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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:O	1:D:157:ILE:CG1	2.59	0.50
1:E:22:SER:N	1:E:91:VAL:HG21	2.26	0.49
1:E:378:GLY:C	1:E:380:LEU:H	2.14	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: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: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: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:B:258:ARG:HB3	1:C:171:ALA:CB	2.44	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:A:356:GLN:HE22	1:B:382:GLN:CD	2.17	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

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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: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: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:C:26:GLU:C	1:C:28:GLU:H	2.18	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
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:A:269:LEU:C	1:A:271:MET:H	2.17	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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: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:C:406:VAL:HG23	1:C:425:PHE:CB	2.45	0.45
1:E:26:GLU:C	1:E:28:GLU:H	2.20	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: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: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: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:E:280:ASN:N	1:E:280:ASN:HD22	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:410:ILE:N	1:D:410:ILE:HD12	2.33	0.44
1:A:212:ALA:HB1	1:A:313:MET:CE	2.48	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: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: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:A:259:ARG:CB	1:B:171:ALA:O	2.67	0.43
1:C:254:ILE:HA	1:C:258:ARG:HD2	2.00	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: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: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: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

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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:A:26:GLU:C	1:A:28:GLU:N	2.71	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:172:ASP:C	1:C:174:ASN:N	2.72	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: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: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
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:B:31:LYS:HE3	1:B:56:ASP:OD1	2.20	0.42
1:C:154:ASP:CG	1:C:155:GLY:N	2.72	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:171:ALA:O	1:A:172:ASP:C	2.59	0.42
1:A:252:GLN:HG2	1:B:190:TYR:OH	2.19	0.42
1:E:173:GLY:O	1:E:174:ASN:CB	2.66	0.42
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:26:GLU:C	1:F:28:GLU:H	2.23	0.41
1:A:212:ALA:HB1	1:A:313:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:269:LEU:C	1:A:271:MET:N	2.74	0.41
1:B:49:TYR:HA	1:B:52:MET:HB3	2.02	0.41
1:C:358:SER:C	1:C:360:GLN:H	2.24	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:269:LEU:C	1:F:271:MET:H	2.23	0.41
1:F:368:ARG:HA	1:F:369:PRO:HD3	1.79	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:150:THR:HG21	1:F:303:ARG:NH2	2.35	0.41
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:D:221:ASP:C	1:D:223:ASP:H	2.24	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:A:358:SER:C	1:A:360:GLN:H	2.23	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:C:269:LEU:C	1:C:271:MET:H	2.22	0.41
1:E:201:ALA:O	1:E:202:ALA:HB2	2.20	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:A:201:ALA:O	1:A:202:ALA:HB2	2.20	0.41
1:B:63:ASP:O	1:B:64:PHE:C	2.58	0.41
1:B:146:GLU:C	1:B:148:SER:H	2.23	0.41
1:B:215:GLN:O	1:B:219:MET:HG3	2.20	0.41
1:B:221:ASP:C	1:B:223:ASP:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:158:ASP:C	1:A:160:ALA:N	2.74	0.40
1:A:367:LYS:HB2	1:A:391:TYR:HE1	1.86	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:F:257:ALA:HB1	1:F:261:PHE:HB3	2.02	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: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:C:206:MET:CE	1:C:391:TYR:HA	2.52	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:B:154:ASP:CG	1:B:155:GLY:N	2.75	0.40
1:C:282:ASN:HA	1:D:157:ILE:CG2	2.52	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%)	3	23
1	B	415/444 (94%)	357 (86%)	47 (11%)	11 (3%)	4	28
1	C	415/444 (94%)	365 (88%)	38 (9%)	12 (3%)	3	27
1	D	403/444 (91%)	355 (88%)	40 (10%)	8 (2%)	6	33
1	E	415/444 (94%)	358 (86%)	43 (10%)	14 (3%)	3	24
1	F	415/444 (94%)	354 (85%)	46 (11%)	15 (4%)	3	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

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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%)	30	54
1	B	361/386 (94%)	343 (95%)	18 (5%)	20	45
1	C	361/386 (94%)	350 (97%)	11 (3%)	36	58
1	D	354/386 (92%)	345 (98%)	9 (2%)	42	62
1	E	361/386 (94%)	346 (96%)	15 (4%)	25	49
1	F	361/386 (94%)	347 (96%)	14 (4%)	27	51
All	All	2159/2316 (93%)	2079 (96%)	80 (4%)	29	53

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

Sometimes 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 oligosaccharides 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, 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%)	1.17	63 (15%) 6 10	103, 118, 142, 151	0
1	B	419/444 (94%)	1.11	65 (15%) 6 9	103, 117, 142, 151	0
1	C	419/444 (94%)	1.33	78 (18%) 4 7	103, 117, 142, 150	0
1	D	409/444 (92%)	1.34	72 (17%) 4 7	103, 117, 142, 150	0
1	E	419/444 (94%)	1.35	87 (20%) 3 6	103, 117, 142, 150	0
1	F	419/444 (94%)	1.23	56 (13%) 8 11	103, 117, 142, 151	0
All	All	2504/2664 (93%)	1.25	421 (16%) 5 8	103, 117, 142, 151	0

All (421) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	SER	6.6
1	C	281	ILE	6.5
1	C	279	SER	6.1
1	A	255	LYS	6.0
1	D	48	ILE	5.4
1	D	157	ILE	5.1
1	E	141	GLU	4.9
1	F	377	SER	4.8
1	C	135	ILE	4.8
1	D	158	ASP	4.8
1	E	134	PRO	4.7
1	E	125	ASN	4.7
1	D	281	ILE	4.7
1	A	376	GLU	4.5
1	F	256	ALA	4.4
1	E	133	LYS	4.4
1	E	135	ILE	4.3
1	D	68	ALA	4.3
1	E	390	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	151	ASP	4.2
1	C	374	LEU	4.2
1	E	162	VAL	4.2
1	C	133	LYS	4.2
1	C	238	ASN	4.1
1	E	32	GLU	4.1
1	A	141	GLU	4.1
1	D	32	GLU	4.1
1	F	160	ALA	4.0
1	B	363	GLN	4.0
1	F	273	ILE	4.0
1	A	123	ASN	3.9
1	D	113	ALA	3.9
1	A	254	ILE	3.9
1	A	133	LYS	3.9
1	D	18	ALA	3.9
1	F	253	LYS	3.8
1	A	251	ALA	3.8
1	F	251	ALA	3.8
1	B	165	TYR	3.8
1	F	165	TYR	3.8
1	F	254	ILE	3.7
1	A	81	PHE	3.7
1	B	287	ALA	3.7
1	D	17	GLN	3.7
1	B	151	ASP	3.7
1	C	251	ALA	3.7
1	B	141	GLU	3.7
1	E	255	LYS	3.6
1	A	270	SER	3.6
1	C	276	ILE	3.6
1	D	22	SER	3.6
1	D	369	PRO	3.6
1	A	256	ALA	3.5
1	D	250	ASN	3.5
1	E	374	LEU	3.5
1	E	252	GLN	3.5
1	D	114	ILE	3.5
1	B	101	CYS	3.5
1	B	152	ASP	3.5
1	C	132	VAL	3.5
1	F	307	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	232	GLU	3.4
1	E	421	VAL	3.4
1	B	255	LYS	3.4
1	E	168	ILE	3.4
1	E	261	PHE	3.4
1	F	257	ALA	3.4
1	A	278	ASN	3.4
1	C	260	ASP	3.4
1	F	144	GLU	3.4
1	A	68	ALA	3.4
1	B	72	GLY	3.4
1	A	157	ILE	3.4
1	D	30	ILE	3.3
1	E	408	VAL	3.3
1	E	138	ALA	3.3
1	C	267	GLY	3.3
1	F	303	ARG	3.3
1	F	258	ARG	3.3
1	D	435	LEU	3.3
1	E	124	VAL	3.3
1	E	389	PHE	3.2
1	F	356	GLN	3.2
1	A	264	GLU	3.2
1	C	272	ALA	3.2
1	A	138	ALA	3.2
1	C	255	LYS	3.2
1	A	158	ASP	3.2
1	C	371	LEU	3.2
1	B	361	VAL	3.2
1	D	261	PHE	3.2
1	C	134	PRO	3.2
1	C	352	ILE	3.1
1	D	283	ILE	3.1
1	E	388	GLU	3.1
1	D	179	PRO	3.1
1	C	409	ILE	3.1
1	E	362	GLU	3.1
1	F	299	ARG	3.1
1	E	121	ILE	3.1
1	E	361	VAL	3.1
1	F	164	VAL	3.1
1	D	76	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	294	ILE	3.1
1	F	252	GLN	3.1
1	B	155	GLY	3.1
1	D	71	VAL	3.1
1	A	92	ALA	3.0
1	B	376	GLU	3.0
1	F	232	GLU	3.0
1	A	377	SER	3.0
1	E	256	ALA	3.0
1	A	267	GLY	3.0
1	E	72	GLY	3.0
1	F	306	PRO	3.0
1	D	160	ALA	3.0
1	A	159	GLU	3.0
1	F	238	ASN	3.0
1	D	253	LYS	3.0
1	A	132	VAL	2.9
1	E	64	PHE	2.9
1	E	132	VAL	2.9
1	F	277	SER	2.9
1	B	92	ALA	2.9
1	F	161	LEU	2.9
1	F	162	VAL	2.9
1	F	159	GLU	2.9
1	D	121	ILE	2.9
1	D	143	MET	2.9
1	F	255	LYS	2.9
1	B	32	GLU	2.9
1	A	260	ASP	2.9
1	A	273	ILE	2.9
1	D	366	ASP	2.9
1	D	262	ALA	2.9
1	E	71	VAL	2.9
1	F	237	GLU	2.9
1	D	255	LYS	2.9
1	D	269	LEU	2.9
1	C	266	TRP	2.9
1	A	232	GLU	2.9
1	C	201	ALA	2.8
1	C	377	SER	2.8
1	E	169	GLU	2.8
1	E	369	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	171	ALA	2.8
1	D	118	GLN	2.8
1	A	173	GLY	2.8
1	A	433	VAL	2.8
1	A	266	TRP	2.8
1	C	193	LYS	2.8
1	D	110	LYS	2.8
1	B	156	SER	2.8
1	D	109	GLN	2.8
1	B	358	SER	2.8
1	C	271	MET	2.8
1	F	261	PHE	2.8
1	E	246	ALA	2.8
1	D	69	ALA	2.8
1	A	135	ILE	2.7
1	D	29	LEU	2.7
1	E	148	SER	2.7
1	B	238	ASN	2.7
1	D	67	ILE	2.7
1	A	373	ASP	2.7
1	D	51	THR	2.7
1	E	113	ALA	2.7
1	F	150	THR	2.7
1	C	424	ALA	2.7
1	A	65	THR	2.7
1	B	65	THR	2.7
1	E	51	THR	2.7
1	C	155	GLY	2.7
1	E	254	ILE	2.7
1	D	246	ALA	2.7
1	D	24	LEU	2.7
1	D	276	ILE	2.7
1	D	374	LEU	2.7
1	E	158	ASP	2.7
1	B	61	SER	2.7
1	F	132	VAL	2.6
1	B	365	GLN	2.6
1	C	313	MET	2.6
1	C	359	ARG	2.6
1	E	373	ASP	2.6
1	C	92	ALA	2.6
1	E	120	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	281	ILE	2.6
1	E	232	GLU	2.6
1	D	395	TYR	2.6
1	F	434	ASN	2.6
1	F	283	ILE	2.6
1	D	380	LEU	2.6
1	E	371	LEU	2.6
1	B	68	ALA	2.6
1	F	267	GLY	2.6
1	D	176	THR	2.5
1	B	263	SER	2.5
1	F	263	SER	2.5
1	D	434	ASN	2.5
1	B	362	GLU	2.5
1	C	141	GLU	2.5
1	E	77	GLN	2.5
1	C	254	ILE	2.5
1	D	135	ILE	2.5
1	E	359	ARG	2.5
1	F	135	ILE	2.5
1	F	345	ARG	2.5
1	C	34	PRO	2.5
1	A	379	GLN	2.5
1	A	415	ASP	2.5
1	E	93	SER	2.5
1	E	208	LYS	2.5
1	C	231	LEU	2.5
1	D	291	VAL	2.5
1	D	390	LEU	2.5
1	E	376	GLU	2.5
1	B	81	PHE	2.5
1	F	422	SER	2.5
1	B	396	TYR	2.5
1	F	141	GLU	2.5
1	C	273	ILE	2.5
1	C	138	ALA	2.5
1	E	79	GLY	2.5
1	A	167	GLU	2.5
1	A	362	GLU	2.5
1	B	157	ILE	2.5
1	E	420	THR	2.4
1	B	367	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	62	VAL	2.4
1	E	350	VAL	2.4
1	E	157	ILE	2.4
1	C	115	SER	2.4
1	C	422	SER	2.4
1	E	146	GLU	2.4
1	E	170	SER	2.4
1	A	174	ASN	2.4
1	C	125	ASN	2.4
1	E	360	GLN	2.4
1	E	74	LYS	2.4
1	A	263	SER	2.4
1	E	348	ASP	2.4
1	E	365	GLN	2.4
1	A	303	ARG	2.4
1	C	29	LEU	2.4
1	C	94	THR	2.4
1	C	247	GLY	2.4
1	C	406	VAL	2.4
1	C	295	TRP	2.4
1	B	264	GLU	2.4
1	E	89	ALA	2.4
1	B	379	GLN	2.4
1	C	372	SER	2.4
1	B	132	VAL	2.4
1	C	249	ILE	2.4
1	D	267	GLY	2.4
1	A	122	GLU	2.4
1	B	89	ALA	2.4
1	B	374	LEU	2.4
1	C	161	LEU	2.4
1	A	153	ASP	2.4
1	A	370	MET	2.4
1	D	65	THR	2.3
1	D	165	TYR	2.3
1	F	14	TYR	2.3
1	A	258	ARG	2.3
1	C	411	ALA	2.3
1	E	45	HIS	2.3
1	D	365	GLN	2.3
1	D	406	VAL	2.3
1	E	145	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	150	THR	2.3
1	F	94	THR	2.3
1	A	371	LEU	2.3
1	B	138	ALA	2.3
1	B	371	LEU	2.3
1	B	230	SER	2.3
1	C	378	GLY	2.3
1	F	316	TYR	2.3
1	A	375	ARG	2.3
1	A	161	LEU	2.3
1	C	361	VAL	2.3
1	F	151	ASP	2.3
1	A	374	LEU	2.3
1	B	266	TRP	2.3
1	C	369	PRO	2.3
1	C	122	GLU	2.3
1	C	144	GLU	2.3
1	D	106	GLU	2.3
1	F	137	GLU	2.3
1	C	139	VAL	2.3
1	D	193	LYS	2.3
1	E	48	ILE	2.3
1	E	139	VAL	2.3
1	C	355	SER	2.3
1	D	213	LEU	2.3
1	F	262	ALA	2.3
1	B	417	PRO	2.3
1	B	409	ILE	2.3
1	D	120	ILE	2.3
1	D	388	GLU	2.3
1	D	97	PHE	2.3
1	C	75	LEU	2.3
1	A	326	ASN	2.3
1	E	315	ASP	2.3
1	A	257	ALA	2.3
1	C	226	VAL	2.2
1	D	62	VAL	2.2
1	F	346	GLU	2.2
1	A	64	PHE	2.2
1	B	99	GLN	2.2
1	B	270	SER	2.2
1	E	61	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	249	ILE	2.2
1	C	228	LEU	2.2
1	B	190	TYR	2.2
1	D	208	LYS	2.2
1	B	93	SER	2.2
1	F	282	ASN	2.2
1	A	435	LEU	2.2
1	E	357	LEU	2.2
1	A	363	GLN	2.2
1	B	382	GLN	2.2
1	E	53	GLN	2.2
1	A	74	LYS	2.2
1	E	411	ALA	2.2
1	A	134	PRO	2.2
1	C	263	SER	2.2
1	F	418	VAL	2.2
1	D	381	GLU	2.2
1	F	269	LEU	2.2
1	B	14	TYR	2.2
1	C	77	GLN	2.2
1	F	363	GLN	2.2
1	E	114	ILE	2.2
1	A	162	VAL	2.2
1	D	361	VAL	2.2
1	C	348	ASP	2.2
1	A	365	GLN	2.2
1	C	14	TYR	2.2
1	B	69	ALA	2.2
1	B	256	ALA	2.2
1	C	389	PHE	2.2
1	F	408	VAL	2.2
1	B	355	SER	2.2
1	C	12	ASN	2.2
1	C	265	ASP	2.2
1	D	238	ASN	2.2
1	C	396	TYR	2.1
1	B	162	VAL	2.1
1	B	87	LEU	2.1
1	E	84	LEU	2.1
1	E	142	LEU	2.1
1	B	33	CYS	2.1
1	E	76	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	193	LYS	2.1
1	D	377	SER	2.1
1	B	316	TYR	2.1
1	C	387	ILE	2.1
1	D	254	ILE	2.1
1	E	409	ILE	2.1
1	C	108	PHE	2.1
1	D	19	VAL	2.1
1	E	406	VAL	2.1
1	E	432	PHE	2.1
1	B	29	LEU	2.1
1	D	125	ASN	2.1
1	A	194	ARG	2.1
1	A	345	ARG	2.1
1	C	145	ILE	2.1
1	E	375	ARG	2.1
1	E	396	TYR	2.1
1	A	411	ALA	2.1
1	D	389	PHE	2.1
1	C	418	VAL	2.1
1	F	136	GLN	2.1
1	F	29	LEU	2.1
1	B	359	ARG	2.1
1	C	157	ILE	2.1
1	C	311	ILE	2.1
1	E	100	HIS	2.1
1	B	27	PRO	2.1
1	A	170	SER	2.1
1	E	395	TYR	2.1
1	C	178	VAL	2.1
1	C	268	LYS	2.1
1	F	304	LYS	2.1
1	A	369	PRO	2.1
1	B	429	TYR	2.1
1	D	107	TYR	2.1
1	E	430	GLY	2.1
1	B	62	VAL	2.1
1	E	310	VAL	2.1
1	C	224	ASP	2.0
1	B	215	GLN	2.0
1	C	289	GLN	2.0
1	F	134	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	183	THR	2.0
1	C	324	LYS	2.0
1	A	429	TYR	2.0
1	D	20	LEU	2.0
1	C	291	VAL	2.0
1	D	117	ALA	2.0
1	E	291	VAL	2.0
1	E	238	ASN	2.0
1	E	358	SER	2.0
1	E	394	ASP	2.0
1	C	356	GLN	2.0
1	F	259	ARG	2.0
1	A	30	ILE	2.0
1	E	281	ILE	2.0
1	D	161	LEU	2.0
1	E	65	THR	2.0
1	E	269	LEU	2.0
1	B	13	GLU	2.0
1	B	15	ALA	2.0
1	F	169	GLU	2.0
1	A	136	GLN	2.0
1	B	345	ARG	2.0
1	C	45	HIS	2.0
1	B	161	LEU	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 monosaccharides 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.