



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 11:46 PM EDT

PDB ID : 6S3U  
Title : Adhesin P140 from Mycoplasma Genitalium  
Authors : Fita, I.; Aparicio, D.  
Deposited on : 2019-06-26  
Resolution : 3.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

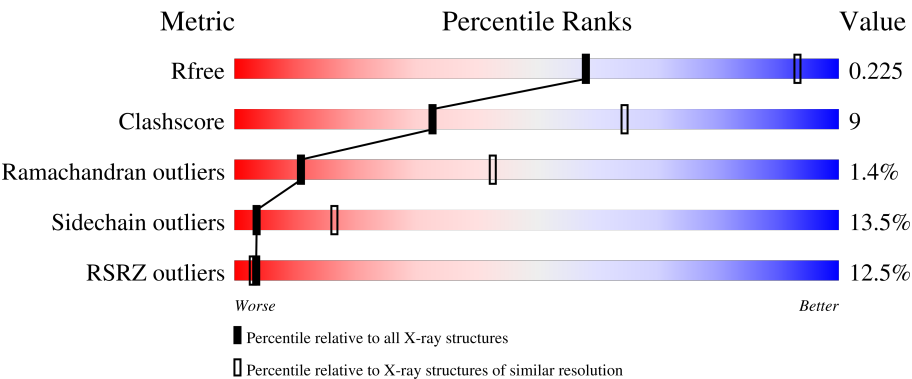
MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 3.24 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 <sub>free</sub>	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1304	<div><div>%</div><div><div></div><div>68%</div><div>26%</div><div>.</div><div>.</div></div></div>
1	B	1304	<div><div>2%</div><div><div></div><div>68%</div><div>26%</div><div>.</div><div>.</div></div></div>
1	C	1304	<div><div>2%</div><div><div></div><div>70%</div><div>25%</div><div>.</div><div>.</div></div></div>
1	D	1304	<div><div>2%</div><div><div></div><div>69%</div><div>24%</div><div>.</div><div>.</div></div></div>
1	E	1304	<div><div>34%</div><div><div></div><div>69%</div><div>24%</div><div>.</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	1304	<div><div></div><div>33%</div><div></div><div>69%</div><div></div><div>24%</div><div></div><div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 59767 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 Adhesin P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1278	Total	C	N	O	S	0	0	0
			10016	6351	1692	1960	13			
1	B	1275	Total	C	N	O	S	0	0	0
			9999	6340	1689	1957	13			
1	C	1274	Total	C	N	O	S	0	0	0
			9993	6339	1688	1953	13			
1	D	1271	Total	C	N	O	S	0	0	0
			9976	6328	1685	1950	13			
1	E	1262	Total	C	N	O	S	0	0	0
			9886	6272	1666	1935	13			
1	F	1262	Total	C	N	O	S	0	0	0
			9897	6281	1668	1935	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1352	HIS	-	expression tag	UNP P20796
A	1353	HIS	-	expression tag	UNP P20796
A	1354	HIS	-	expression tag	UNP P20796
A	1355	HIS	-	expression tag	UNP P20796
A	1356	HIS	-	expression tag	UNP P20796
A	1357	HIS	-	expression tag	UNP P20796
B	1352	HIS	-	expression tag	UNP P20796
B	1353	HIS	-	expression tag	UNP P20796
B	1354	HIS	-	expression tag	UNP P20796
B	1355	HIS	-	expression tag	UNP P20796
B	1356	HIS	-	expression tag	UNP P20796
B	1357	HIS	-	expression tag	UNP P20796
C	1352	HIS	-	expression tag	UNP P20796
C	1353	HIS	-	expression tag	UNP P20796
C	1354	HIS	-	expression tag	UNP P20796
C	1355	HIS	-	expression tag	UNP P20796
C	1356	HIS	-	expression tag	UNP P20796

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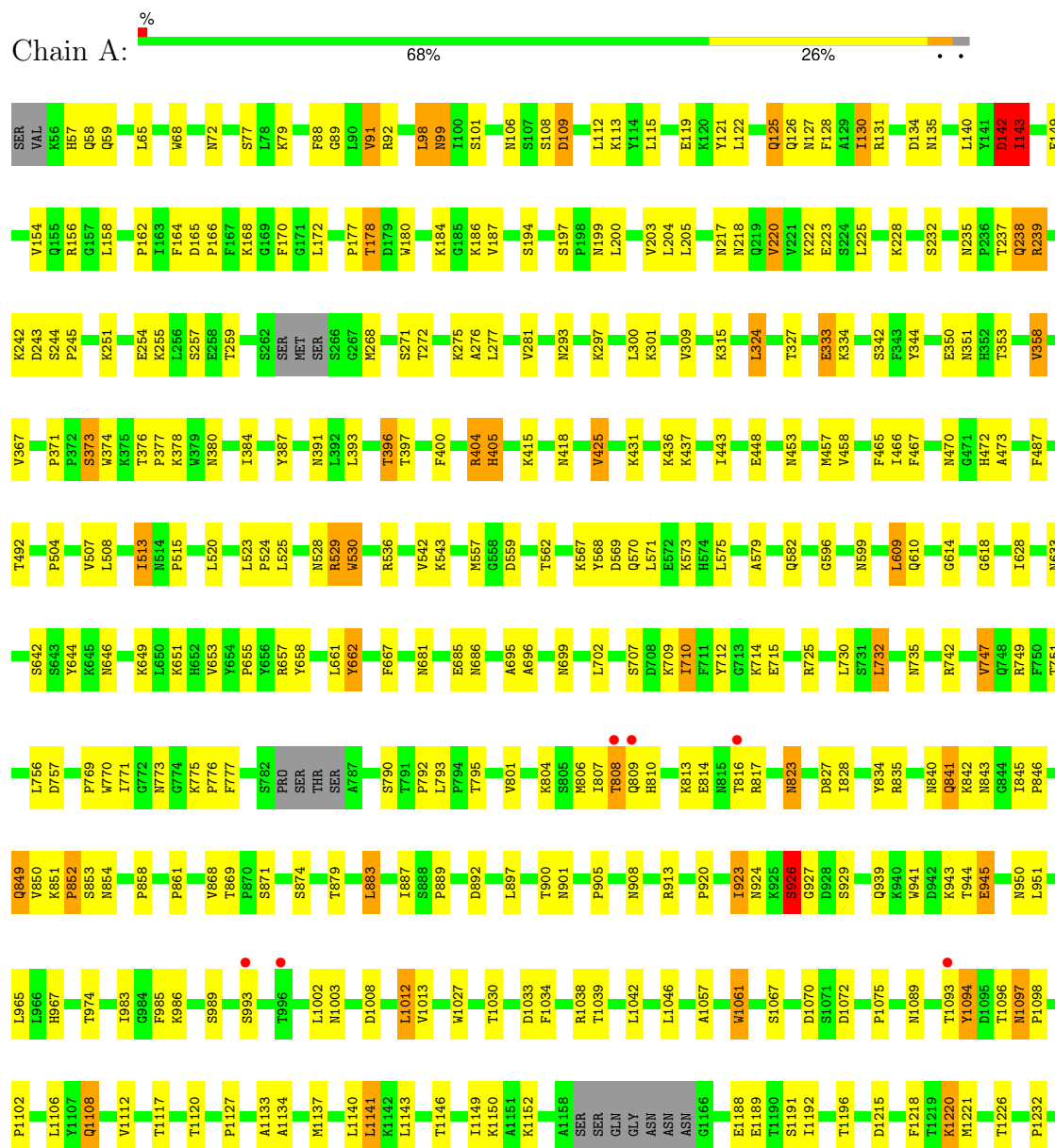
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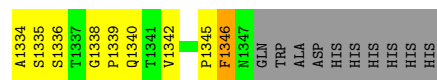
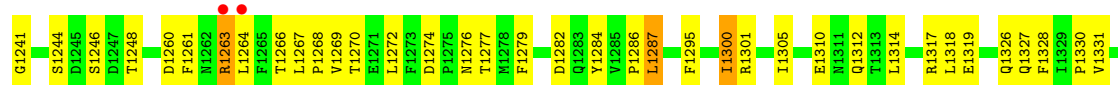
Chain	Residue	Modelled	Actual	Comment	Reference
C	1357	HIS	-	expression tag	UNP P20796
D	1352	HIS	-	expression tag	UNP P20796
D	1353	HIS	-	expression tag	UNP P20796
D	1354	HIS	-	expression tag	UNP P20796
D	1355	HIS	-	expression tag	UNP P20796
D	1356	HIS	-	expression tag	UNP P20796
D	1357	HIS	-	expression tag	UNP P20796
E	1352	HIS	-	expression tag	UNP P20796
E	1353	HIS	-	expression tag	UNP P20796
E	1354	HIS	-	expression tag	UNP P20796
E	1355	HIS	-	expression tag	UNP P20796
E	1356	HIS	-	expression tag	UNP P20796
E	1357	HIS	-	expression tag	UNP P20796
F	1352	HIS	-	expression tag	UNP P20796
F	1353	HIS	-	expression tag	UNP P20796
F	1354	HIS	-	expression tag	UNP P20796
F	1355	HIS	-	expression tag	UNP P20796
F	1356	HIS	-	expression tag	UNP P20796
F	1357	HIS	-	expression tag	UNP P20796

### 3 Residue-property plots

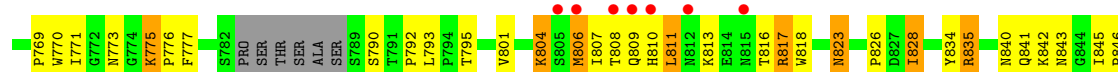
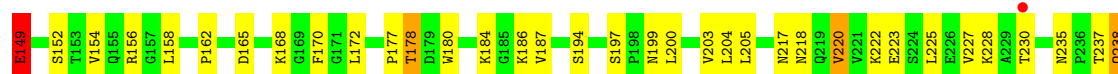
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

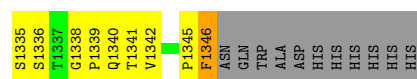
#### • Molecule 1: Adhesin P1



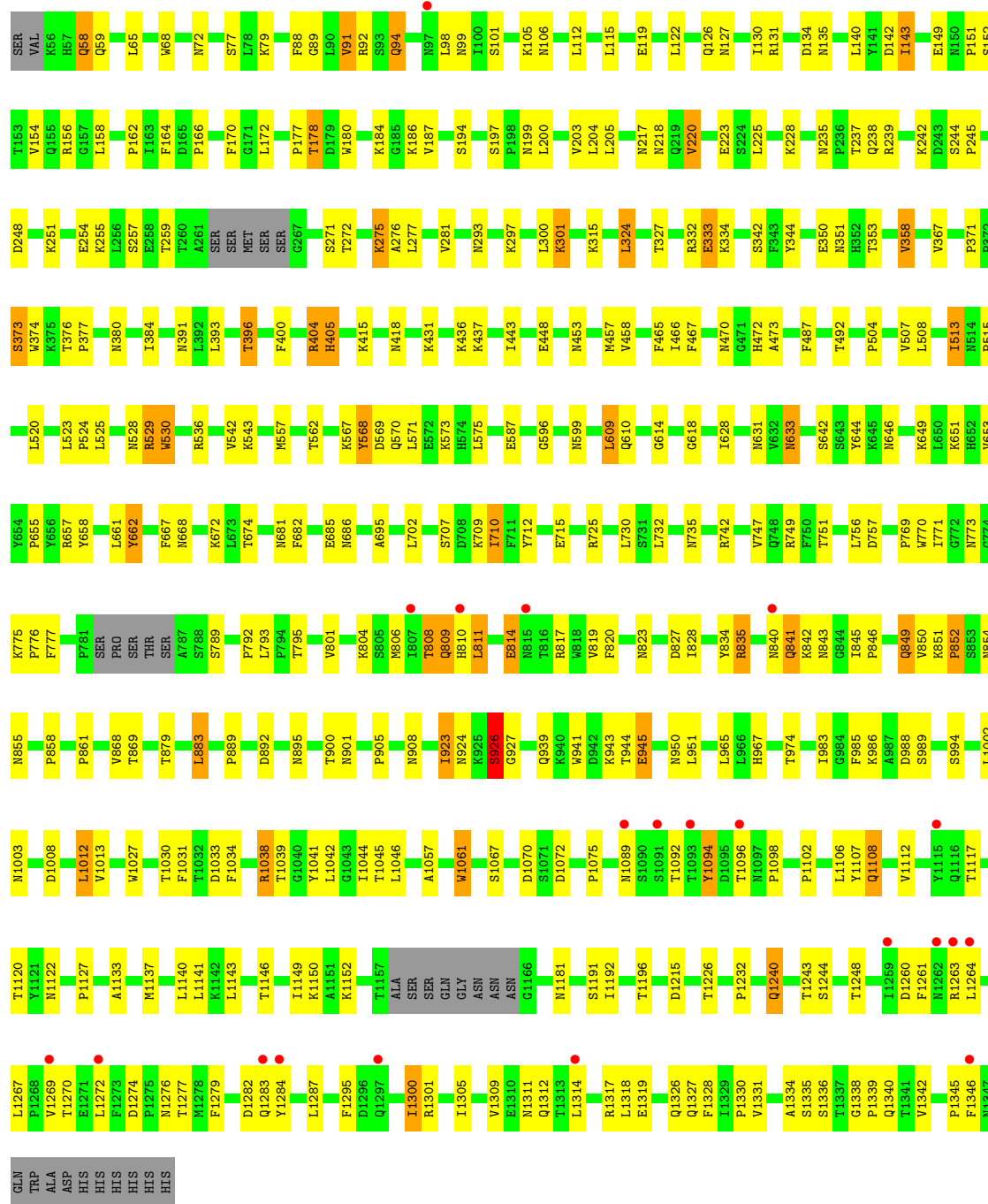


### • Molecule 1: Adhesin P1





● Molecule 1: Adhesin P1

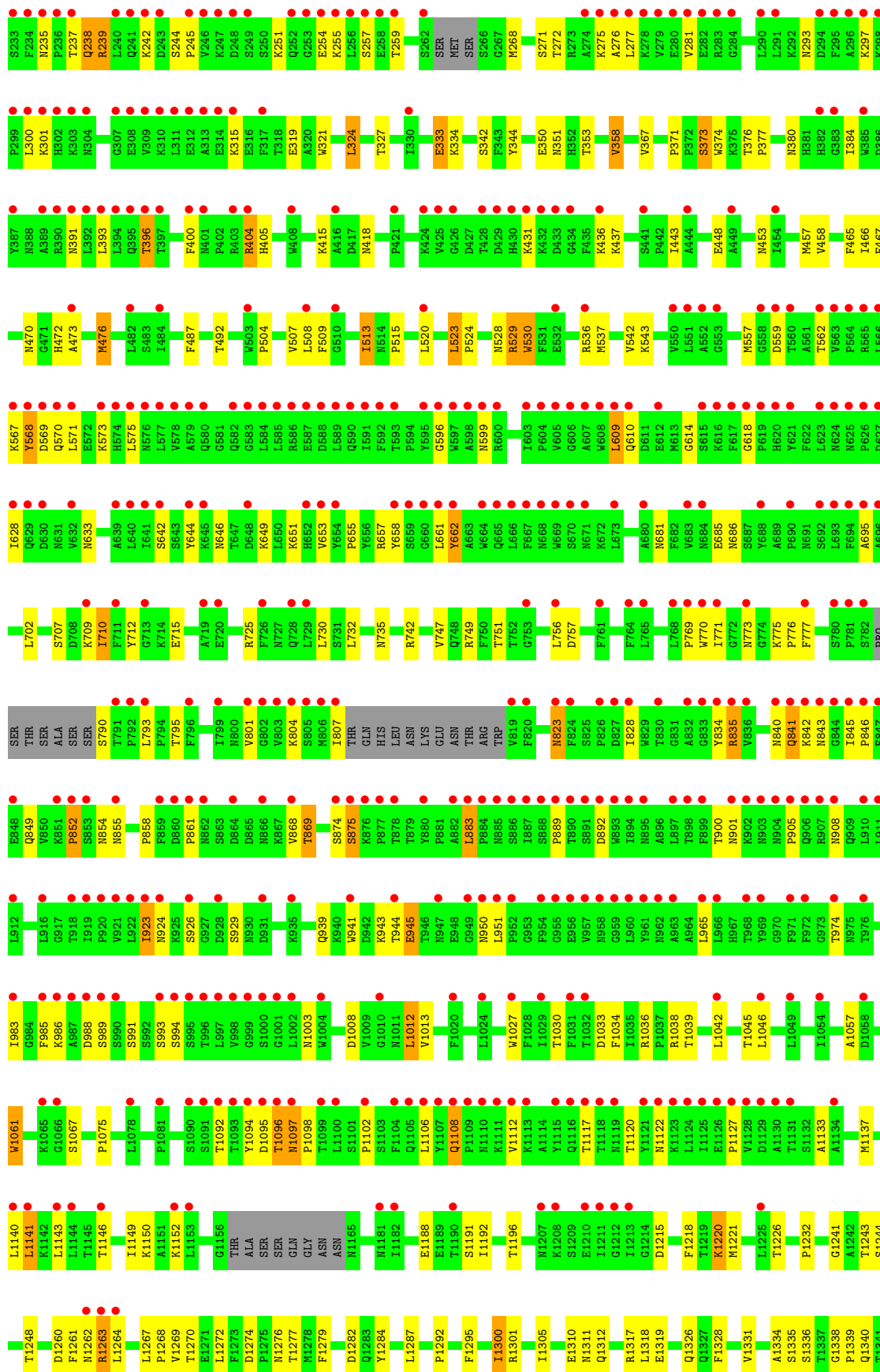


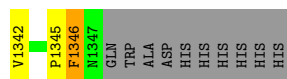
● Molecule 1: Adhesin P1



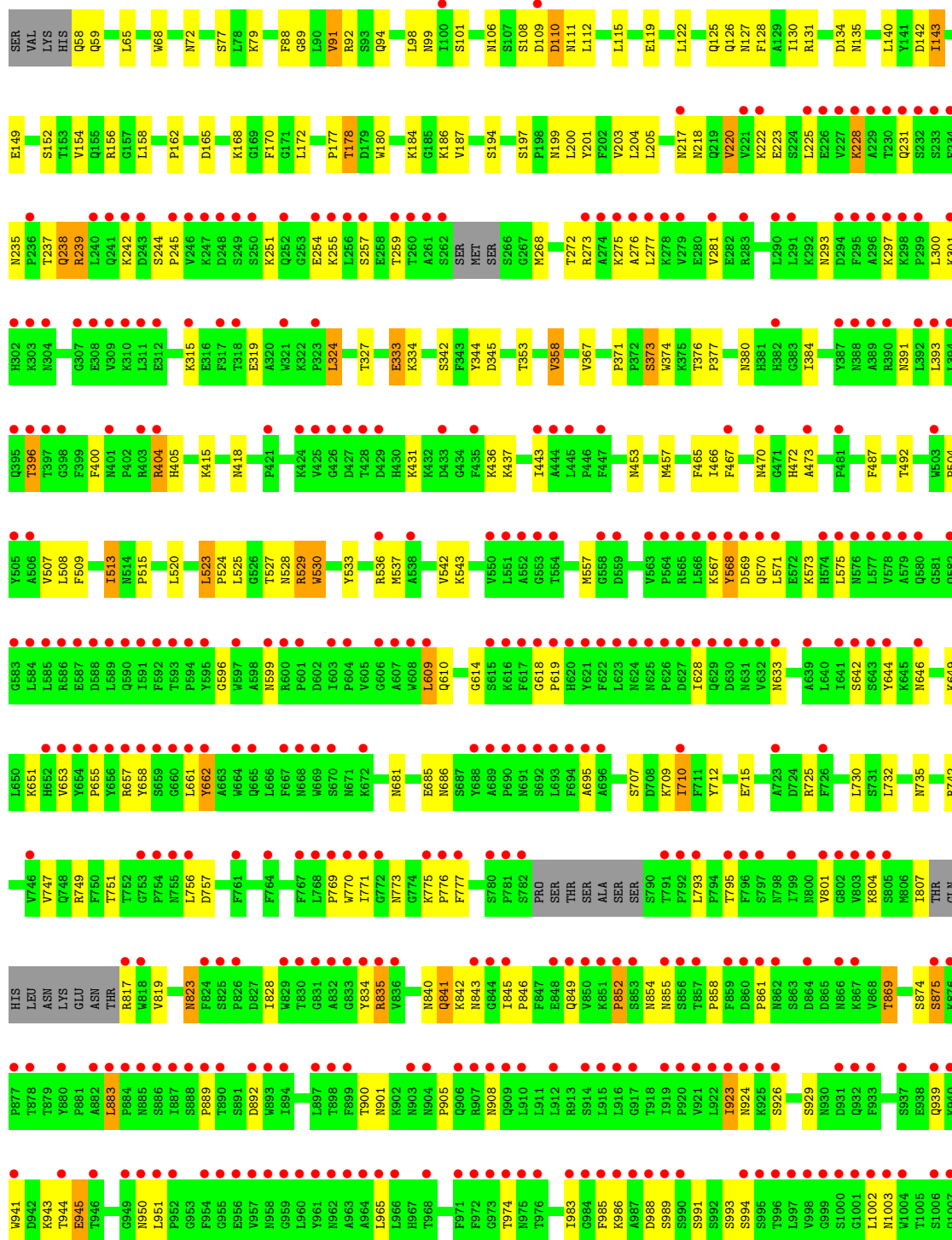


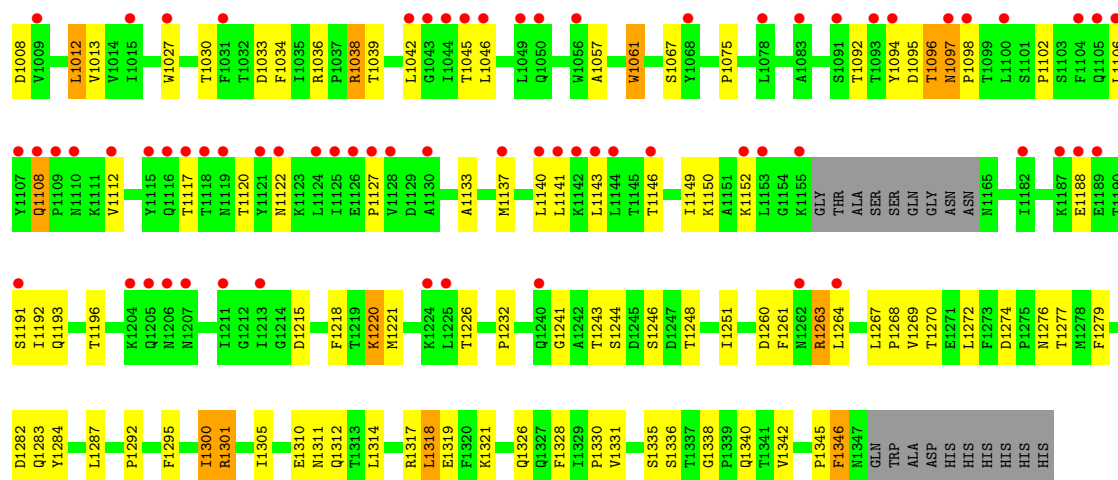






● Molecule 1: Adhesin P1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	459.19Å 116.66Å 285.64Å 90.00° 124.20° 90.00°	Depositor
Resolution (Å)	37.36 – 3.24 236.25 – 3.24	Depositor EDS
% Data completeness (in resolution range)	61.7 (37.36-3.24) 61.8 (236.25-3.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 3.26Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.184 , 0.205 0.202 , 0.225	Depositor DCC
$R_{free}$ test set	6155 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 96.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	59767	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.52	0/10269	0.78	6/13978 (0.0%)
1	B	0.49	0/10252	0.76	3/13956 (0.0%)
1	C	0.50	0/10246	0.76	1/13947 (0.0%)
1	D	0.50	0/10229	0.76	3/13925 (0.0%)
1	E	0.45	0/10135	0.73	2/13795 (0.0%)
1	F	0.45	0/10147	0.73	2/13812 (0.0%)
All	All	0.49	0/61278	0.75	17/83413 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	476	MET	CB-CG-SD	7.17	133.92	112.40
1	E	861	PRO	N-CA-C	-6.71	94.65	112.10
1	F	861	PRO	N-CA-C	-6.65	94.81	112.10
1	A	109	ASP	C-N-CA	6.20	137.21	121.70
1	A	806	MET	C-N-CA	6.17	137.12	121.70
1	A	143	ILE	N-CA-C	-5.86	95.19	111.00
1	B	849	GLN	C-N-CA	5.72	136.00	121.70
1	D	849	GLN	C-N-CA	5.72	136.00	121.70
1	B	853	SER	C-N-CA	5.62	135.76	121.70
1	D	1174	ASN	C-N-CA	5.61	135.73	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	849	GLN	C-N-CA	5.58	135.65	121.70
1	A	849	GLN	C-N-CA	5.53	135.51	121.70
1	A	1093	THR	C-N-CA	5.40	135.21	121.70
1	B	149	GLU	N-CA-C	-5.34	96.58	111.00
1	F	110	ASP	C-N-CA	5.28	134.91	121.70
1	A	142	ASP	N-CA-C	-5.14	97.12	111.00
1	D	812	ASN	C-N-CA	5.13	134.53	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	926	SER	Mainchain
1	C	926	SER	Mainchain

## 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	10016	0	9726	182	0
1	B	9999	0	9707	183	0
1	C	9993	0	9706	182	0
1	D	9976	0	9687	205	0
1	E	9886	0	9597	156	0
1	F	9897	0	9610	163	0
All	All	59767	0	58033	1029	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 9.

All (1029) 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:100:ILE:CG1	1:D:100:ILE:CD1	1.76	1.57
1:D:812:ASN:ND2	1:D:815:ASN:HD22	1.28	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1279:PHE:CE2	1:F:1301:ARG:HD2	1.78	1.18
1:A:1266:THR:HG21	1:C:1264:LEU:HD11	1.19	1.15
1:A:1264:LEU:HG	1:C:1283:GLN:HB2	1.30	1.09
1:F:1279:PHE:HE2	1:F:1301:ARG:HD2	1.09	1.05
1:C:1279:PHE:CE2	1:C:1301:ARG:HD2	1.93	1.02
1:F:1279:PHE:CE2	1:F:1301:ARG:CD	2.42	1.01
1:D:812:ASN:ND2	1:D:815:ASN:ND2	2.09	1.00
1:D:1279:PHE:CE1	1:D:1301:ARG:HD2	2.00	0.96
1:E:1279:PHE:CE1	1:E:1301:ARG:HD2	2.00	0.96
1:A:1287:LEU:HD22	1:D:158:LEU:HD21	1.46	0.96
1:B:1279:PHE:CE1	1:B:1301:ARG:HD2	2.01	0.96
1:A:1279:PHE:CE1	1:A:1301:ARG:HD2	2.01	0.93
1:F:1301:ARG:HG2	1:F:1328:PHE:CE2	2.03	0.92
1:A:528:ASN:HD22	1:A:530:TRP:HE3	1.15	0.92
1:F:1301:ARG:HG2	1:F:1328:PHE:CD2	2.04	0.92
1:E:528:ASN:HD22	1:E:530:TRP:HE3	1.17	0.90
1:F:528:ASN:HD22	1:F:530:TRP:HE3	1.17	0.90
1:C:667:PHE:HE2	1:D:815:ASN:O	1.53	0.90
1:C:808:THR:HB	1:D:634:ASN:OD1	1.72	0.90
1:C:528:ASN:HD22	1:C:530:TRP:HE3	1.18	0.89
1:D:528:ASN:HD22	1:D:530:TRP:HE3	1.18	0.89
1:D:277:LEU:HD13	1:D:620:HIS:NE2	1.87	0.89
1:B:528:ASN:HD22	1:B:530:TRP:HE3	1.17	0.89
1:B:277:LEU:HD13	1:B:620:HIS:NE2	1.89	0.88
1:A:387:TYR:CE2	1:A:425:VAL:HG21	2.09	0.87
1:D:812:ASN:HD21	1:D:815:ASN:HD22	1.21	0.87
1:D:813:LYS:H	1:D:817:ARG:HH12	1.23	0.86
1:A:1134:ALA:HA	1:A:1137:MET:CE	2.07	0.85
1:C:667:PHE:CE2	1:D:815:ASN:O	2.29	0.85
1:A:1274:ASP:HB3	1:A:1277:THR:HG22	1.59	0.84
1:F:1274:ASP:HB3	1:F:1277:THR:HG22	1.58	0.84
1:A:1264:LEU:HD13	1:A:1284:TYR:HE1	1.42	0.83
1:D:1274:ASP:HB3	1:D:1277:THR:HG22	1.60	0.83
1:E:1274:ASP:HB3	1:E:1277:THR:HG22	1.60	0.83
1:B:1226:THR:H	1:B:1238:ASN:HD21	1.25	0.83
1:B:1274:ASP:HB3	1:B:1277:THR:HG22	1.59	0.83
1:A:1266:THR:CG2	1:C:1264:LEU:HD11	2.07	0.82
1:C:1274:ASP:HB3	1:C:1277:THR:HG22	1.63	0.80
1:E:1264:LEU:HD13	1:E:1284:TYR:HE2	1.47	0.80
1:C:674:THR:HG21	1:D:814:GLU:OE2	1.81	0.80
1:A:1134:ALA:HA	1:A:1137:MET:HE2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASP:HB2	1:A:113:LYS:HD2	1.64	0.79
1:C:820:PHE:HE2	1:D:682:PHE:HE2	1.30	0.79
1:B:237:THR:HG22	1:B:1108:GLN:HG3	1.66	0.78
1:C:1264:LEU:HD13	1:C:1284:TYR:HE1	1.47	0.77
1:F:1264:LEU:HD13	1:F:1284:TYR:HE1	1.49	0.77
1:A:1264:LEU:HG	1:C:1283:GLN:CB	2.13	0.76
1:E:237:THR:HG22	1:E:1108:GLN:HG3	1.68	0.76
1:F:237:THR:HG22	1:F:1108:GLN:HG3	1.68	0.76
1:C:237:THR:HG22	1:C:1108:GLN:HG3	1.68	0.75
1:D:237:THR:HG22	1:D:1108:GLN:HG3	1.69	0.75
1:D:810:HIS:CG	1:D:818:TRP:CZ3	2.76	0.74
1:A:1097:ASN:HB3	1:A:1098:PRO:CD	2.17	0.74
1:B:1264:LEU:HD13	1:B:1284:TYR:HE1	1.52	0.74
1:D:811:LEU:CD1	1:D:894:ILE:HG13	2.17	0.74
1:D:1264:LEU:HD13	1:D:1284:TYR:HE1	1.52	0.73
1:D:813:LYS:H	1:D:817:ARG:NH1	1.86	0.73
1:D:813:LYS:N	1:D:817:ARG:HH12	1.87	0.73
1:E:869:THR:HG23	1:E:875:SER:H	1.54	0.72
1:A:237:THR:HG22	1:A:1108:GLN:HG3	1.69	0.72
1:D:1097:ASN:HB2	1:D:1098:PRO:HD3	1.70	0.72
1:A:528:ASN:ND2	1:A:530:TRP:HE3	1.86	0.72
1:C:1279:PHE:HE2	1:C:1301:ARG:HD2	1.48	0.72
1:E:528:ASN:ND2	1:E:530:TRP:HE3	1.88	0.71
1:F:869:THR:HG23	1:F:875:SER:H	1.53	0.71
1:B:923:ILE:HG22	1:B:1140:LEU:HD23	1.72	0.71
1:C:528:ASN:ND2	1:C:530:TRP:HE3	1.88	0.71
1:D:1305:ILE:HD11	1:D:1317:ARG:HB3	1.73	0.71
1:A:923:ILE:HG22	1:A:1140:LEU:HD23	1.72	0.71
1:B:617:PHE:CD2	1:B:859:PHE:HD2	2.09	0.71
1:C:820:PHE:HE2	1:D:682:PHE:CE2	2.09	0.71
1:D:923:ILE:HG22	1:D:1140:LEU:HD23	1.72	0.71
1:B:987:ALA:HB1	1:B:1115:TYR:CD2	2.25	0.71
1:D:528:ASN:ND2	1:D:530:TRP:HE3	1.89	0.71
1:A:1264:LEU:HD13	1:A:1284:TYR:CE1	2.25	0.70
1:B:528:ASN:ND2	1:B:530:TRP:HE3	1.89	0.70
1:D:810:HIS:CD2	1:D:818:TRP:CZ3	2.79	0.70
1:C:769:PRO:HA	1:C:776:PRO:HA	1.74	0.69
1:A:98:LEU:HD12	1:A:125:GLN:HG2	1.73	0.69
1:A:109:ASP:CB	1:A:113:LYS:HD2	2.22	0.69
1:A:387:TYR:HE2	1:A:425:VAL:HG21	1.58	0.69
1:D:194:SER:HB2	1:D:200:LEU:HD23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:923:ILE:HG22	1:F:1140:LEU:HD23	1.75	0.69
1:A:1305:ILE:HD11	1:A:1317:ARG:HB3	1.75	0.68
1:B:769:PRO:HA	1:B:776:PRO:HA	1.76	0.68
1:B:1305:ILE:HD11	1:B:1317:ARG:HB3	1.74	0.68
1:B:277:LEU:HD13	1:B:620:HIS:CD2	2.29	0.68
1:C:923:ILE:HG22	1:C:1140:LEU:HD23	1.74	0.68
1:F:1305:ILE:HD11	1:F:1317:ARG:HB3	1.75	0.68
1:F:769:PRO:HA	1:F:776:PRO:HA	1.76	0.68
1:E:194:SER:HB2	1:E:200:LEU:HD23	1.76	0.68
1:A:1287:LEU:HD22	1:D:158:LEU:CD2	2.21	0.67
1:F:528:ASN:ND2	1:F:530:TRP:HE3	1.89	0.67
1:F:988:ASP:OD2	1:F:991:SER:O	2.12	0.67
1:F:194:SER:HB2	1:F:200:LEU:HD23	1.75	0.67
1:A:1266:THR:HG21	1:C:1264:LEU:CD1	2.13	0.67
1:C:1264:LEU:HD13	1:C:1284:TYR:CE1	2.28	0.67
1:E:923:ILE:HG22	1:E:1140:LEU:HD23	1.76	0.67
1:A:769:PRO:HA	1:A:776:PRO:HA	1.76	0.67
1:F:1263:ARG:HG3	1:F:1264:LEU:HD12	1.76	0.67
1:E:1264:LEU:HD13	1:E:1284:TYR:CE2	2.30	0.67
1:E:1305:ILE:HD11	1:E:1317:ARG:HB3	1.76	0.67
1:B:1263:ARG:HG3	1:B:1264:LEU:HD12	1.77	0.67
1:B:194:SER:HB2	1:B:200:LEU:HD23	1.77	0.66
1:A:1263:ARG:HG3	1:A:1264:LEU:HD12	1.78	0.66
1:D:1263:ARG:HG3	1:D:1264:LEU:HD12	1.77	0.66
1:A:809:GLN:HG2	1:B:634:ASN:HB2	1.76	0.66
1:C:1305:ILE:HD11	1:C:1317:ARG:HB3	1.77	0.66
1:C:570:GLN:HG2	1:C:596:GLY:HA2	1.77	0.66
1:E:1263:ARG:HG3	1:E:1264:LEU:HD12	1.77	0.66
1:D:769:PRO:HA	1:D:776:PRO:HA	1.76	0.66
1:D:617:PHE:CD2	1:D:859:PHE:HD2	2.14	0.65
1:E:646:ASN:HB2	1:F:823:ASN:HA	1.77	0.65
1:E:988:ASP:OD2	1:E:991:SER:O	2.13	0.65
1:A:570:GLN:HG2	1:A:596:GLY:HA2	1.78	0.65
1:E:769:PRO:HA	1:E:776:PRO:HA	1.77	0.65
1:D:95:ASN:HD21	1:D:125:GLN:HG3	1.62	0.65
1:F:1264:LEU:HD13	1:F:1284:TYR:CE1	2.31	0.65
1:A:194:SER:HB2	1:A:200:LEU:HD23	1.79	0.65
1:C:194:SER:HB2	1:C:200:LEU:HD23	1.78	0.65
1:B:777:PHE:O	1:B:795:THR:HG22	1.98	0.64
1:A:1097:ASN:HB3	1:A:1098:PRO:HD3	1.80	0.64
1:D:277:LEU:HD13	1:D:620:HIS:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:PHE:O	1:A:795:THR:HG22	1.98	0.63
1:D:217:ASN:HB3	1:D:220:VAL:HG23	1.80	0.63
1:D:244:SER:HB2	1:D:568:TYR:O	1.99	0.63
1:B:570:GLN:HG2	1:B:596:GLY:HA2	1.80	0.63
1:D:1264:LEU:HD13	1:D:1284:TYR:CE1	2.33	0.63
1:F:570:GLN:HG2	1:F:596:GLY:HA2	1.80	0.63
1:B:217:ASN:HB3	1:B:220:VAL:HG23	1.81	0.63
1:C:820:PHE:CE2	1:D:682:PHE:HE2	2.13	0.63
1:B:681:ASN:HB2	1:B:730:LEU:HD22	1.80	0.63
1:D:570:GLN:HG2	1:D:596:GLY:HA2	1.79	0.63
1:B:58:GLN:NE2	1:B:149:GLU:O	2.32	0.63
1:C:777:PHE:O	1:C:795:THR:HG22	1.99	0.63
1:C:1263:ARG:HG3	1:C:1264:LEU:HD12	1.80	0.63
1:A:244:SER:HB3	1:A:571:LEU:HB2	1.80	0.62
1:D:777:PHE:O	1:D:795:THR:HG22	1.99	0.62
1:B:244:SER:HB3	1:B:571:LEU:HB2	1.82	0.62
1:B:1264:LEU:HD13	1:B:1284:TYR:CE1	2.33	0.62
1:D:812:ASN:HD21	1:D:815:ASN:ND2	1.86	0.62
1:A:808:THR:HB	1:B:634:ASN:OD1	1.99	0.62
1:C:809:GLN:HE22	1:C:811:LEU:HD23	1.64	0.62
1:E:777:PHE:O	1:E:795:THR:HG22	2.00	0.62
1:F:1279:PHE:CE2	1:F:1301:ARG:HD3	2.33	0.62
1:B:834:TYR:OH	1:B:945:GLU:HG2	2.00	0.62
1:C:681:ASN:HB2	1:C:730:LEU:HD22	1.80	0.62
1:F:79:LYS:HD3	1:F:1232:PRO:HA	1.82	0.62
1:C:244:SER:HB3	1:C:571:LEU:HB2	1.82	0.62
1:E:1003:ASN:HB3	1:E:1102:PRO:HG2	1.82	0.62
1:B:244:SER:HB2	1:B:568:TYR:O	2.00	0.61
1:A:1003:ASN:HB3	1:A:1102:PRO:HG2	1.82	0.61
1:B:1248:THR:HB	1:B:1331:VAL:HG13	1.82	0.61
1:E:1279:PHE:HE1	1:E:1301:ARG:HD2	1.64	0.61
1:E:570:GLN:HG2	1:E:596:GLY:HA2	1.81	0.61
1:B:1033:ASP:OD1	1:B:1038:ARG:HG3	1.99	0.61
1:C:1248:THR:HB	1:C:1331:VAL:HG13	1.83	0.61
1:D:1248:THR:HB	1:D:1331:VAL:HG13	1.82	0.61
1:C:217:ASN:HB3	1:C:220:VAL:HG23	1.82	0.61
1:E:244:SER:HB3	1:E:571:LEU:HB2	1.82	0.61
1:E:79:LYS:HD3	1:E:1232:PRO:HA	1.83	0.61
1:C:244:SER:HB2	1:C:568:TYR:O	2.01	0.61
1:A:1248:THR:HB	1:A:1331:VAL:HG13	1.83	0.61
1:C:1033:ASP:OD1	1:C:1038:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1248:THR:HB	1:F:1331:VAL:HG13	1.83	0.61
1:A:217:ASN:HB3	1:A:220:VAL:HG23	1.82	0.61
1:C:811:LEU:HD11	1:C:895:ASN:O	2.01	0.61
1:F:244:SER:HB2	1:F:568:TYR:O	2.01	0.61
1:F:244:SER:HB3	1:F:571:LEU:HB2	1.82	0.61
1:F:1301:ARG:HG2	1:F:1328:PHE:HD2	1.63	0.61
1:F:777:PHE:O	1:F:795:THR:HG22	2.00	0.60
1:B:277:LEU:HD13	1:B:620:HIS:HE2	1.66	0.60
1:C:1003:ASN:HB3	1:C:1102:PRO:HG2	1.83	0.60
1:D:244:SER:HB3	1:D:571:LEU:HB2	1.83	0.60
1:D:935:LYS:HB3	1:D:972:PHE:HD2	1.66	0.60
1:D:1003:ASN:HB3	1:D:1102:PRO:HG2	1.84	0.60
1:E:742:ARG:HH12	1:F:1036:ARG:HH21	1.50	0.60
1:A:244:SER:HB2	1:A:568:TYR:O	2.01	0.60
1:D:79:LYS:HD3	1:D:1232:PRO:HA	1.84	0.60
1:E:852:PRO:HA	1:E:858:PRO:HA	1.84	0.60
1:F:1003:ASN:HB3	1:F:1102:PRO:HG2	1.83	0.60
1:C:94:GLN:HA	1:C:94:GLN:HE21	1.67	0.59
1:C:457:MET:HA	1:C:465:PHE:O	2.02	0.59
1:C:817:ARG:HG2	1:C:817:ARG:HH21	1.67	0.59
1:E:457:MET:HA	1:E:465:PHE:O	2.02	0.59
1:F:217:ASN:HB3	1:F:220:VAL:HG23	1.84	0.59
1:A:79:LYS:HD3	1:A:1232:PRO:HA	1.85	0.59
1:C:105:LYS:HZ2	1:C:105:LYS:HB2	1.66	0.59
1:D:614:GLY:HA3	1:D:854:ASN:HD21	1.67	0.59
1:F:457:MET:HA	1:F:465:PHE:O	2.01	0.59
1:E:244:SER:HB2	1:E:568:TYR:O	2.02	0.59
1:A:1134:ALA:HA	1:A:1137:MET:HE1	1.83	0.59
1:C:810:HIS:NE2	1:C:814:GLU:HA	2.18	0.59
1:F:1301:ARG:HG2	1:F:1328:PHE:HE2	1.64	0.59
1:B:457:MET:HA	1:B:465:PHE:O	2.02	0.59
1:D:834:TYR:OH	1:D:945:GLU:HG2	2.03	0.59
1:F:1033:ASP:OD1	1:F:1038:ARG:HG3	2.02	0.59
1:A:817:ARG:HG2	1:A:817:ARG:HH21	1.68	0.59
1:B:1003:ASN:HB3	1:B:1102:PRO:HG2	1.85	0.58
1:E:217:ASN:HB3	1:E:220:VAL:HG23	1.84	0.58
1:C:122:LEU:HB3	1:C:126:GLN:HE21	1.68	0.58
1:E:742:ARG:HH12	1:F:1036:ARG:NH2	2.01	0.58
1:A:681:ASN:HB2	1:A:730:LEU:HD22	1.85	0.58
1:A:852:PRO:HA	1:A:858:PRO:HA	1.85	0.58
1:C:852:PRO:HA	1:C:858:PRO:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:PHE:CE2	1:B:816:THR:HG23	2.38	0.58
1:A:59:GLN:HB2	1:A:142:ASP:O	2.03	0.58
1:D:457:MET:HA	1:D:465:PHE:O	2.03	0.58
1:D:811:LEU:HA	1:D:817:ARG:HH11	1.67	0.58
1:F:852:PRO:HA	1:F:858:PRO:HA	1.84	0.58
1:B:79:LYS:HD3	1:B:1232:PRO:HA	1.85	0.58
1:F:681:ASN:HB2	1:F:730:LEU:HD22	1.86	0.58
1:E:681:ASN:HB2	1:E:730:LEU:HD22	1.85	0.58
1:A:457:MET:HA	1:A:465:PHE:O	2.04	0.58
1:C:513:ILE:HD12	1:C:515:PRO:HD2	1.86	0.58
1:D:813:LYS:HA	1:D:817:ARG:HH12	1.69	0.58
1:F:1261:PHE:HE1	1:F:1345:PRO:HA	1.69	0.57
1:B:852:PRO:HA	1:B:858:PRO:HA	1.85	0.57
1:D:646:ASN:HD22	1:D:651:LYS:HA	1.70	0.57
1:D:809:GLN:CG	1:D:894:ILE:HG21	2.34	0.57
1:C:105:LYS:HB2	1:C:105:LYS:NZ	2.19	0.57
1:D:852:PRO:HA	1:D:858:PRO:HA	1.87	0.57
1:B:804:LYS:H	1:B:804:LYS:HD3	1.70	0.57
1:C:834:TYR:OH	1:C:945:GLU:HG2	2.05	0.57
1:D:95:ASN:ND2	1:D:125:GLN:HG3	2.18	0.57
1:D:277:LEU:HD13	1:D:620:HIS:HE2	1.64	0.57
1:E:834:TYR:OH	1:E:945:GLU:HG2	2.05	0.57
1:C:939:GLN:HE21	1:C:950:ASN:HD22	1.53	0.57
1:B:1295:PHE:HE2	1:B:1300:ILE:HG12	1.69	0.57
1:C:79:LYS:HD3	1:C:1232:PRO:HA	1.86	0.57
1:C:819:VAL:HG23	1:C:820:PHE:HD1	1.70	0.57
1:D:614:GLY:HA3	1:D:854:ASN:ND2	2.20	0.57
1:F:58:GLN:OE1	1:F:149:GLU:HB3	2.04	0.56
1:F:834:TYR:OH	1:F:945:GLU:HG2	2.04	0.56
1:C:674:THR:CG2	1:D:814:GLU:OE2	2.52	0.56
1:D:804:LYS:H	1:D:804:LYS:HD3	1.68	0.56
1:A:646:ASN:HD22	1:A:651:LYS:HA	1.71	0.56
1:C:199:ASN:O	1:C:344:TYR:HA	2.05	0.56
1:D:681:ASN:HB2	1:D:730:LEU:HD22	1.86	0.56
1:D:1295:PHE:HE2	1:D:1300:ILE:HG12	1.69	0.56
1:C:1096:THR:HG22	1:C:1098:PRO:HD2	1.87	0.56
1:A:834:TYR:OH	1:A:945:GLU:HG2	2.05	0.56
1:A:939:GLN:HE21	1:A:950:ASN:HD22	1.53	0.56
1:C:820:PHE:CE2	1:D:682:PHE:CE2	2.93	0.56
1:E:1295:PHE:HE2	1:E:1300:ILE:HG12	1.71	0.56
1:F:646:ASN:HD22	1:F:651:LYS:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:LEU:CG	1:C:1283:GLN:HB2	2.20	0.56
1:B:646:ASN:HD22	1:B:651:LYS:HA	1.71	0.56
1:C:646:ASN:HD22	1:C:651:LYS:HA	1.71	0.56
1:D:513:ILE:HD12	1:D:515:PRO:HD2	1.86	0.56
1:F:1335:SER:HB3	1:F:1338:GLY:O	2.06	0.56
1:D:1030:THR:HB	1:D:1045:THR:OG1	2.06	0.56
1:D:122:LEU:HB3	1:D:126:GLN:HE21	1.71	0.56
1:E:1248:THR:HB	1:E:1331:VAL:HG13	1.86	0.56
1:B:1261:PHE:HE1	1:B:1345:PRO:HA	1.71	0.55
1:E:646:ASN:HD22	1:E:651:LYS:HA	1.71	0.55
1:F:1218:PHE:HE2	1:F:1220:LYS:HG2	1.71	0.55
1:B:770:TRP:HE3	1:B:773:ASN:HB2	1.71	0.55
1:E:58:GLN:OE1	1:E:149:GLU:HB3	2.05	0.55
1:E:255:LYS:HD2	1:E:609:LEU:HB2	1.89	0.55
1:A:255:LYS:HD2	1:A:609:LEU:HB2	1.89	0.55
1:A:813:LYS:HA	1:B:817:ARG:HG2	1.88	0.55
1:E:695:ALA:HB3	1:E:751:THR:HG22	1.89	0.55
1:F:134:ASP:HB3	1:F:140:LEU:HD21	1.89	0.55
1:F:695:ALA:HB3	1:F:751:THR:HG22	1.89	0.55
1:F:939:GLN:HE21	1:F:950:ASN:HD22	1.55	0.55
1:D:813:LYS:CA	1:D:817:ARG:HH12	2.18	0.55
1:B:1115:TYR:HE1	1:B:1125:ILE:HG21	1.72	0.55
1:A:122:LEU:HB3	1:A:126:GLN:HE21	1.71	0.55
1:C:255:LYS:HD2	1:C:609:LEU:HB2	1.88	0.55
1:F:770:TRP:HE3	1:F:773:ASN:HB2	1.72	0.55
1:A:77:SER:HA	1:A:89:GLY:HA2	1.89	0.54
1:B:199:ASN:O	1:B:344:TYR:HA	2.07	0.54
1:C:1030:THR:HB	1:C:1045:THR:OG1	2.07	0.54
1:A:770:TRP:HE3	1:A:773:ASN:HB2	1.72	0.54
1:B:1335:SER:HB3	1:B:1338:GLY:O	2.07	0.54
1:E:1335:SER:HB3	1:E:1338:GLY:O	2.07	0.54
1:F:255:LYS:HD2	1:F:609:LEU:HB2	1.88	0.54
1:A:1295:PHE:HE2	1:A:1300:ILE:HG12	1.71	0.54
1:E:68:TRP:CD1	1:E:92:ARG:HB2	2.43	0.54
1:A:58:GLN:OE1	1:A:149:GLU:HB3	2.06	0.54
1:B:924:ASN:HB2	1:B:985:PHE:HA	1.90	0.54
1:D:770:TRP:HE3	1:D:773:ASN:HB2	1.72	0.54
1:E:134:ASP:HB3	1:E:140:LEU:HD21	1.89	0.54
1:C:614:GLY:HA3	1:C:854:ASN:HD21	1.73	0.54
1:A:199:ASN:O	1:A:344:TYR:HA	2.07	0.54
1:A:1335:SER:HB3	1:A:1338:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1335:SER:HB3	1:C:1338:GLY:O	2.08	0.54
1:F:122:LEU:HB3	1:F:126:GLN:HE21	1.73	0.54
1:C:924:ASN:HB2	1:C:985:PHE:HA	1.89	0.54
1:E:770:TRP:HE3	1:E:773:ASN:HB2	1.72	0.54
1:E:939:GLN:HE21	1:E:950:ASN:HD22	1.55	0.54
1:B:65:LEU:HB3	1:B:91:VAL:HG13	1.90	0.54
1:E:823:ASN:HA	1:F:646:ASN:HB2	1.90	0.54
1:B:122:LEU:HB3	1:B:126:GLN:HE21	1.72	0.53
1:E:199:ASN:O	1:E:344:TYR:HA	2.08	0.53
1:F:1295:PHE:HE2	1:F:1300:ILE:HG12	1.72	0.53
1:B:1143:LEU:HD23	1:B:1149:ILE:HG12	1.89	0.53
1:B:1030:THR:HB	1:B:1045:THR:OG1	2.08	0.53
1:A:529:ARG:HB2	1:A:715:GLU:O	2.08	0.53
1:A:1218:PHE:HE2	1:A:1220:LYS:HG2	1.73	0.53
1:D:134:ASP:HB3	1:D:140:LEU:HD21	1.91	0.53
1:E:321:TRP:HE1	1:E:476:MET:CE	2.21	0.53
1:A:134:ASP:HB3	1:A:140:LEU:HD21	1.91	0.53
1:B:939:GLN:HE21	1:B:950:ASN:HD22	1.55	0.53
1:E:524:PRO:HD2	1:E:557:MET:HE2	1.90	0.53
1:B:1218:PHE:HE2	1:B:1220:LYS:HG2	1.73	0.53
1:C:77:SER:HA	1:C:89:GLY:HA2	1.91	0.53
1:C:614:GLY:HA3	1:C:854:ASN:ND2	2.24	0.53
1:C:770:TRP:HE3	1:C:773:ASN:HB2	1.73	0.53
1:D:924:ASN:HB2	1:D:985:PHE:HA	1.89	0.53
1:E:1218:PHE:HE2	1:E:1220:LYS:HG2	1.73	0.53
1:D:255:LYS:HD2	1:D:609:LEU:HB2	1.90	0.53
1:B:134:ASP:HB3	1:B:140:LEU:HD21	1.90	0.53
1:B:695:ALA:HB3	1:B:751:THR:HG22	1.91	0.53
1:C:668:ASN:ND2	1:D:816:THR:OG1	2.36	0.53
1:D:812:ASN:H	1:D:817:ARG:HH11	1.56	0.53
1:D:846:PRO:HG2	1:D:849:GLN:HE22	1.73	0.53
1:C:1143:LEU:HD23	1:C:1149:ILE:HG12	1.91	0.53
1:D:939:GLN:HE21	1:D:950:ASN:HD22	1.56	0.53
1:F:65:LEU:HB3	1:F:91:VAL:HG13	1.91	0.53
1:F:924:ASN:HB2	1:F:985:PHE:HA	1.91	0.53
1:A:924:ASN:HB2	1:A:985:PHE:HA	1.91	0.52
1:C:134:ASP:HB3	1:C:140:LEU:HD21	1.91	0.52
1:D:396:THR:HG21	1:D:404:ARG:HE	1.75	0.52
1:E:1030:THR:HB	1:E:1045:THR:OG1	2.09	0.52
1:F:817:ARG:HG2	1:F:817:ARG:HH21	1.73	0.52
1:A:513:ILE:HD12	1:A:515:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:695:ALA:HB3	1:D:751:THR:HG22	1.92	0.52
1:C:808:THR:CB	1:D:634:ASN:OD1	2.53	0.52
1:D:1335:SER:HB3	1:D:1338:GLY:O	2.09	0.52
1:E:77:SER:HA	1:E:89:GLY:HA2	1.91	0.52
1:E:924:ASN:HB2	1:E:985:PHE:HA	1.91	0.52
1:F:513:ILE:HD12	1:F:515:PRO:HD2	1.91	0.52
1:F:1030:THR:HB	1:F:1045:THR:OG1	2.09	0.52
1:B:255:LYS:HD2	1:B:609:LEU:HB2	1.90	0.52
1:C:248:ASP:HB2	1:C:301:LYS:HB2	1.92	0.52
1:D:199:ASN:O	1:D:344:TYR:HA	2.08	0.52
1:E:1003:ASN:HD21	1:E:1146:THR:HG21	1.74	0.52
1:F:199:ASN:O	1:F:344:TYR:HA	2.09	0.52
1:D:816:THR:HB	1:D:819:VAL:HG22	1.92	0.52
1:D:1218:PHE:HE2	1:D:1220:LYS:HG2	1.73	0.52
1:C:846:PRO:HG2	1:C:849:GLN:HE22	1.73	0.52
1:C:892:ASP:HA	1:C:900:THR:HG23	1.92	0.52
1:D:248:ASP:HB2	1:D:301:LYS:HB2	1.92	0.52
1:B:228:LYS:HE2	1:B:230:THR:HB	1.91	0.52
1:B:248:ASP:HB2	1:B:301:LYS:HB2	1.92	0.52
1:D:1313:THR:HG22	1:D:1344:GLN:HG3	1.91	0.52
1:A:695:ALA:HB3	1:A:751:THR:HG22	1.92	0.51
1:C:1295:PHE:HE2	1:C:1300:ILE:HG12	1.73	0.51
1:F:68:TRP:CD1	1:F:92:ARG:HB2	2.45	0.51
1:F:846:PRO:HG2	1:F:849:GLN:HE22	1.74	0.51
1:A:68:TRP:CD1	1:A:92:ARG:HB2	2.45	0.51
1:B:529:ARG:HB2	1:B:715:GLU:O	2.10	0.51
1:D:77:SER:HA	1:D:89:GLY:HA2	1.92	0.51
1:D:529:ARG:HB2	1:D:715:GLU:O	2.10	0.51
1:D:809:GLN:HG3	1:D:894:ILE:HG21	1.92	0.51
1:E:846:PRO:HG2	1:E:849:GLN:HE22	1.74	0.51
1:A:65:LEU:HB3	1:A:91:VAL:HG13	1.92	0.51
1:B:846:PRO:HG2	1:B:849:GLN:HE22	1.74	0.51
1:C:695:ALA:HB3	1:C:751:THR:HG22	1.91	0.51
1:F:529:ARG:HB2	1:F:715:GLU:O	2.09	0.51
1:B:59:GLN:HB2	1:B:143:ILE:H	1.76	0.51
1:F:1003:ASN:HD21	1:F:1146:THR:HG21	1.76	0.51
1:A:1261:PHE:HE1	1:A:1345:PRO:HA	1.76	0.51
1:B:68:TRP:CD1	1:B:92:ARG:HB2	2.46	0.51
1:E:513:ILE:HD12	1:E:515:PRO:HD2	1.93	0.51
1:A:897:LEU:CD2	1:B:816:THR:HG21	2.41	0.51
1:B:834:TYR:CZ	1:B:945:GLU:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1003:ASN:HD21	1:C:1146:THR:HG21	1.76	0.51
1:E:122:LEU:HB3	1:E:126:GLN:HE21	1.74	0.51
1:B:1014:VAL:O	1:B:1069:LEU:HD22	2.11	0.51
1:C:529:ARG:HB2	1:C:715:GLU:O	2.11	0.51
1:B:817:ARG:HB3	1:B:818:TRP:CD1	2.46	0.51
1:D:58:GLN:OE1	1:D:149:GLU:HB3	2.11	0.51
1:D:65:LEU:HB3	1:D:91:VAL:HG13	1.93	0.50
1:D:834:TYR:CZ	1:D:945:GLU:HG2	2.47	0.50
1:F:77:SER:HA	1:F:89:GLY:HA2	1.93	0.50
1:B:112:LEU:HD11	1:B:333:GLU:HG2	1.92	0.50
1:D:68:TRP:CD1	1:D:92:ARG:HB2	2.46	0.50
1:F:1027:TRP:CE3	1:F:1046:LEU:HB3	2.47	0.50
1:A:1003:ASN:HD21	1:A:1146:THR:HG21	1.75	0.50
1:C:65:LEU:HB3	1:C:91:VAL:HG13	1.92	0.50
1:D:809:GLN:HG3	1:D:894:ILE:CG2	2.41	0.50
1:E:529:ARG:HB2	1:E:715:GLU:O	2.10	0.50
1:E:834:TYR:CZ	1:E:945:GLU:HG2	2.47	0.50
1:B:892:ASP:HA	1:B:900:THR:HG23	1.93	0.50
1:C:98:LEU:O	1:C:98:LEU:HD12	2.11	0.50
1:D:186:LYS:HB3	1:D:205:LEU:HB3	1.94	0.50
1:A:154:VAL:HG23	1:A:170:PHE:HB3	1.94	0.50
1:A:504:PRO:HG2	1:A:507:VAL:HG23	1.94	0.50
1:E:1027:TRP:CE3	1:E:1046:LEU:HB3	2.46	0.50
1:E:1261:PHE:HE1	1:E:1345:PRO:HA	1.77	0.50
1:F:523:LEU:HG	1:F:557:MET:CE	2.42	0.50
1:A:377:PRO:HG3	1:A:443:ILE:HG13	1.94	0.50
1:A:396:THR:HG21	1:A:404:ARG:HE	1.76	0.50
1:A:892:ASP:HA	1:A:900:THR:HG23	1.93	0.50
1:A:1027:TRP:CE3	1:A:1046:LEU:HB3	2.46	0.50
1:B:513:ILE:HD12	1:B:515:PRO:HD2	1.93	0.50
1:B:869:THR:HG22	1:B:875:SER:OG	2.11	0.50
1:C:1261:PHE:HE1	1:C:1345:PRO:HA	1.76	0.50
1:D:276:ALA:HB2	1:D:655:PRO:HD3	1.93	0.50
1:D:810:HIS:CD2	1:D:818:TRP:HZ3	2.26	0.50
1:E:614:GLY:HA3	1:E:854:ASN:HD21	1.77	0.50
1:E:742:ARG:NH1	1:F:1036:ARG:HH21	2.09	0.50
1:C:1027:TRP:CE3	1:C:1046:LEU:HB3	2.46	0.50
1:A:186:LYS:HB3	1:A:205:LEU:HB3	1.94	0.50
1:A:254:GLU:O	1:A:297:LYS:HB3	2.12	0.50
1:C:396:THR:HG21	1:C:404:ARG:HE	1.77	0.50
1:C:674:THR:CB	1:D:814:GLU:OE2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:892:ASP:HA	1:E:900:THR:HG23	1.93	0.50
1:F:892:ASP:HA	1:F:900:THR:HG23	1.93	0.50
1:F:254:GLU:O	1:F:297:LYS:HB3	2.12	0.49
1:E:371:PRO:HD2	1:E:374:TRP:CD2	2.47	0.49
1:B:77:SER:HA	1:B:89:GLY:HA2	1.94	0.49
1:B:396:THR:HG21	1:B:404:ARG:HE	1.77	0.49
1:E:65:LEU:HB3	1:E:91:VAL:HG13	1.92	0.49
1:E:321:TRP:HE1	1:E:476:MET:HE3	1.78	0.49
1:A:926:SER:O	1:A:983:ILE:HG12	2.12	0.49
1:B:813:LYS:HA	1:B:817:ARG:HH22	1.78	0.49
1:C:254:GLU:O	1:C:297:LYS:HB3	2.12	0.49
1:F:614:GLY:HA3	1:F:854:ASN:HD21	1.77	0.49
1:A:112:LEU:HD11	1:A:333:GLU:HG2	1.93	0.49
1:A:327:THR:HG21	1:A:367:VAL:HG21	1.95	0.49
1:A:834:TYR:CZ	1:A:945:GLU:HG2	2.48	0.49
1:B:1226:THR:H	1:B:1238:ASN:ND2	2.03	0.49
1:C:58:GLN:OE1	1:C:149:GLU:HB3	2.13	0.49
1:C:834:TYR:CZ	1:C:945:GLU:HG2	2.47	0.49
1:D:327:THR:HG21	1:D:367:VAL:HG21	1.94	0.49
1:D:812:ASN:H	1:D:817:ARG:NH1	2.10	0.49
1:D:1143:LEU:HD23	1:D:1149:ILE:HG12	1.95	0.49
1:E:59:GLN:HB2	1:E:143:ILE:H	1.78	0.49
1:A:1143:LEU:HD23	1:A:1149:ILE:HG12	1.94	0.49
1:D:112:LEU:HD11	1:D:333:GLU:HG2	1.93	0.49
1:A:846:PRO:HG2	1:A:849:GLN:HE22	1.77	0.49
1:C:68:TRP:CD1	1:C:92:ARG:HB2	2.47	0.49
1:B:1003:ASN:HD21	1:B:1146:THR:HG21	1.77	0.49
1:C:391:ASN:HD22	1:C:418:ASN:HD22	1.61	0.49
1:D:811:LEU:CD1	1:D:894:ILE:CG1	2.88	0.49
1:D:1027:TRP:CE3	1:D:1046:LEU:HB3	2.47	0.49
1:F:777:PHE:HB3	1:F:795:THR:CG2	2.43	0.49
1:A:98:LEU:O	1:A:99:ASN:C	2.49	0.49
1:B:466:ILE:HB	1:B:487:PHE:HB2	1.94	0.49
1:C:371:PRO:HD2	1:C:374:TRP:CD2	2.48	0.49
1:C:994:SER:HB2	1:C:1137:MET:CE	2.42	0.49
1:D:254:GLU:O	1:D:297:LYS:HB3	2.12	0.49
1:D:275:LYS:HG2	1:D:644:TYR:HE1	1.78	0.49
1:B:186:LYS:HB3	1:B:205:LEU:HB3	1.95	0.49
1:B:987:ALA:HA	1:B:1115:TYR:CE2	2.48	0.49
1:E:466:ILE:HB	1:E:487:PHE:HB2	1.95	0.49
1:E:994:SER:HB2	1:E:1137:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:396:THR:HG21	1:F:404:ARG:HE	1.78	0.49
1:D:777:PHE:HB3	1:D:795:THR:CG2	2.43	0.48
1:B:994:SER:HB2	1:B:1137:MET:HE3	1.95	0.48
1:C:777:PHE:HB3	1:C:795:THR:CG2	2.43	0.48
1:E:1143:LEU:HD23	1:E:1149:ILE:HG12	1.95	0.48
1:F:59:GLN:HB2	1:F:143:ILE:H	1.78	0.48
1:F:834:TYR:CZ	1:F:945:GLU:HG2	2.47	0.48
1:D:391:ASN:HD22	1:D:418:ASN:HD22	1.62	0.48
1:A:651:LYS:CE	1:B:823:ASN:HD21	2.26	0.48
1:B:987:ALA:CB	1:B:1115:TYR:CD2	2.96	0.48
1:E:112:LEU:HD11	1:E:333:GLU:HG2	1.95	0.48
1:B:809:GLN:HB3	1:B:826:PRO:HB2	1.95	0.48
1:C:277:LEU:HB2	1:C:653:VAL:HB	1.96	0.48
1:D:1003:ASN:HD21	1:D:1146:THR:HG21	1.79	0.48
1:E:154:VAL:HG23	1:E:170:PHE:HB3	1.96	0.48
1:E:777:PHE:HB3	1:E:795:THR:CG2	2.44	0.48
1:A:98:LEU:O	1:A:121:TYR:OH	2.31	0.48
1:B:617:PHE:CE2	1:B:859:PHE:HB2	2.48	0.48
1:B:1312:GLN:O	1:B:1345:PRO:HD2	2.13	0.48
1:C:466:ILE:HB	1:C:487:PHE:HB2	1.95	0.48
1:C:1143:LEU:O	1:C:1149:ILE:HD11	2.14	0.48
1:F:276:ALA:HB2	1:F:655:PRO:HD3	1.96	0.48
1:A:1097:ASN:CB	1:A:1098:PRO:CD	2.90	0.48
1:D:994:SER:HB2	1:D:1137:MET:CE	2.43	0.48
1:F:523:LEU:HG	1:F:557:MET:HE2	1.96	0.48
1:A:277:LEU:HB2	1:A:653:VAL:HB	1.96	0.48
1:B:58:GLN:OE1	1:B:149:GLU:HB3	2.13	0.48
1:B:520:LEU:HD23	1:B:757:ASP:HA	1.95	0.48
1:C:186:LYS:HB3	1:C:205:LEU:HB3	1.96	0.48
1:D:154:VAL:HG23	1:D:170:PHE:HB3	1.95	0.48
1:D:892:ASP:HA	1:D:900:THR:HG23	1.95	0.48
1:F:112:LEU:HD11	1:F:333:GLU:HG2	1.96	0.48
1:E:254:GLU:O	1:E:297:LYS:HB3	2.13	0.48
1:F:1312:GLN:O	1:F:1345:PRO:HD2	2.14	0.48
1:B:806:MET:HB2	1:B:843:ASN:OD1	2.13	0.48
1:B:994:SER:HB2	1:B:1137:MET:CE	2.44	0.48
1:B:1027:TRP:CE3	1:B:1046:LEU:HB3	2.48	0.48
1:C:889:PRO:HD2	1:C:951:LEU:HD21	1.95	0.48
1:E:523:LEU:HB3	1:E:557:MET:HE1	1.96	0.48
1:F:377:PRO:HB2	1:F:400:PHE:O	2.14	0.48
1:C:154:VAL:HG23	1:C:170:PHE:HB3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ALA:HB2	1:C:655:PRO:HD3	1.96	0.47
1:C:377:PRO:HG3	1:C:443:ILE:HG13	1.95	0.47
1:E:396:THR:HG21	1:E:404:ARG:HE	1.79	0.47
1:A:245:PRO:HG2	1:A:568:TYR:HB2	1.96	0.47
1:C:327:THR:HG21	1:C:367:VAL:HG21	1.96	0.47
1:D:371:PRO:HD2	1:D:374:TRP:CD2	2.49	0.47
1:F:186:LYS:HB3	1:F:205:LEU:HB3	1.96	0.47
1:A:391:ASN:HD22	1:A:418:ASN:HD22	1.62	0.47
1:B:276:ALA:HB2	1:B:655:PRO:HD3	1.96	0.47
1:B:377:PRO:HB2	1:B:400:PHE:O	2.14	0.47
1:C:112:LEU:HD11	1:C:333:GLU:HG2	1.96	0.47
1:E:231:GLN:HG3	1:E:1096:THR:HA	1.97	0.47
1:F:371:PRO:HD2	1:F:374:TRP:CD2	2.48	0.47
1:F:994:SER:HB2	1:F:1137:MET:CE	2.43	0.47
1:C:245:PRO:HG2	1:C:568:TYR:HB2	1.97	0.47
1:C:520:LEU:HD23	1:C:757:ASP:HA	1.97	0.47
1:C:845:ILE:HG22	1:C:883:LEU:O	2.15	0.47
1:E:276:ALA:HB2	1:E:655:PRO:HD3	1.96	0.47
1:F:277:LEU:HB2	1:F:653:VAL:HB	1.96	0.47
1:A:614:GLY:HA3	1:A:854:ASN:HD21	1.80	0.47
1:B:254:GLU:O	1:B:297:LYS:HB3	2.14	0.47
1:D:59:GLN:HB2	1:D:143:ILE:H	1.79	0.47
1:F:377:PRO:HG3	1:F:443:ILE:HG13	1.97	0.47
1:A:277:LEU:HD21	1:A:610:GLN:HG3	1.97	0.47
1:B:777:PHE:HB3	1:B:795:THR:CG2	2.45	0.47
1:D:811:LEU:HD13	1:D:894:ILE:HG13	1.95	0.47
1:B:277:LEU:HD21	1:B:610:GLN:CG	2.45	0.47
1:E:186:LYS:HB3	1:E:205:LEU:HB3	1.97	0.47
1:E:277:LEU:HB2	1:E:653:VAL:HB	1.96	0.47
1:E:377:PRO:HB2	1:E:400:PHE:O	2.15	0.47
1:E:520:LEU:HD23	1:E:757:ASP:HA	1.96	0.47
1:E:614:GLY:HA3	1:E:854:ASN:ND2	2.30	0.47
1:A:777:PHE:HB3	1:A:795:THR:CG2	2.45	0.47
1:C:793:LEU:HD22	1:C:801:VAL:HG13	1.96	0.47
1:D:889:PRO:HD2	1:D:951:LEU:HD21	1.96	0.47
1:F:1261:PHE:CE1	1:F:1345:PRO:HA	2.50	0.47
1:A:570:GLN:HG2	1:A:596:GLY:CA	2.45	0.47
1:B:178:THR:O	1:B:358:VAL:HG11	2.15	0.47
1:B:391:ASN:HD22	1:B:418:ASN:HD22	1.62	0.47
1:E:889:PRO:HD2	1:E:951:LEU:HD21	1.97	0.47
1:E:1036:ARG:HH21	1:F:742:ARG:HH12	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:LEU:O	1:A:1149:ILE:HD11	2.16	0.46
1:C:377:PRO:HB2	1:C:400:PHE:O	2.15	0.46
1:A:178:THR:O	1:A:358:VAL:HG11	2.15	0.46
1:A:371:PRO:HD2	1:A:374:TRP:CD2	2.50	0.46
1:A:466:ILE:HB	1:A:487:PHE:HB2	1.96	0.46
1:A:1013:VAL:HG11	1:A:1075:PRO:HB3	1.98	0.46
1:B:154:VAL:HG23	1:B:170:PHE:HB3	1.96	0.46
1:B:275:LYS:HG3	1:B:644:TYR:HE1	1.81	0.46
1:D:520:LEU:HD23	1:D:757:ASP:HA	1.97	0.46
1:E:448:GLU:H	1:E:448:GLU:HG2	1.48	0.46
1:F:1143:LEU:HD23	1:F:1149:ILE:HG12	1.95	0.46
1:A:559:ASP:OD2	1:A:562:THR:HB	2.16	0.46
1:E:1143:LEU:O	1:E:1149:ILE:HD11	2.15	0.46
1:F:889:PRO:HD2	1:F:951:LEU:HD21	1.97	0.46
1:B:1345:PRO:O	1:B:1346:PHE:HB2	2.15	0.46
1:D:845:ILE:HG22	1:D:883:LEU:O	2.16	0.46
1:A:770:TRP:CE3	1:A:773:ASN:HB2	2.51	0.46
1:A:793:LEU:HD22	1:A:801:VAL:HG13	1.97	0.46
1:B:277:LEU:HB2	1:B:653:VAL:HB	1.98	0.46
1:B:327:THR:HG21	1:B:367:VAL:HG21	1.97	0.46
1:B:373:SER:HB2	1:B:374:TRP:HD1	1.79	0.46
1:C:570:GLN:HG2	1:C:596:GLY:CA	2.46	0.46
1:C:710:ILE:HD11	1:C:712:TYR:CZ	2.49	0.46
1:C:1191:SER:HB2	1:C:1196:THR:HG23	1.98	0.46
1:E:228:LYS:NZ	1:E:1096:THR:HG21	2.30	0.46
1:E:327:THR:HG21	1:E:367:VAL:HG21	1.97	0.46
1:E:1036:ARG:NH2	1:F:742:ARG:HH12	2.13	0.46
1:A:92:ARG:HG3	1:A:128:PHE:CE1	2.51	0.46
1:C:945:GLU:H	1:C:945:GLU:HG3	1.24	0.46
1:D:277:LEU:HD21	1:D:610:GLN:CG	2.45	0.46
1:F:162:PRO:HG3	1:F:344:TYR:CE2	2.51	0.46
1:A:275:LYS:HG3	1:A:644:TYR:HE1	1.81	0.46
1:A:276:ALA:HB2	1:A:655:PRO:HD3	1.97	0.46
1:F:614:GLY:HA3	1:F:854:ASN:ND2	2.31	0.46
1:A:983:ILE:HD11	1:A:1152:LYS:HD2	1.98	0.46
1:C:281:VAL:HG22	1:C:293:ASN:HA	1.98	0.46
1:D:281:VAL:HG22	1:D:293:ASN:HA	1.98	0.46
1:D:373:SER:HB2	1:D:374:TRP:HD1	1.81	0.46
1:E:177:PRO:HG2	1:E:180:TRP:CE3	2.51	0.46
1:F:1143:LEU:O	1:F:1149:ILE:HD11	2.15	0.46
1:A:377:PRO:HB2	1:A:400:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1286:PRO:HG2	1:D:158:LEU:HD22	1.97	0.46
1:D:817:ARG:N	1:D:817:ARG:HD2	2.30	0.46
1:E:275:LYS:HG3	1:E:644:TYR:HE1	1.81	0.46
1:E:504:PRO:HG2	1:E:507:VAL:HG23	1.97	0.46
1:F:245:PRO:HG2	1:F:568:TYR:HB2	1.98	0.46
1:F:504:PRO:HG2	1:F:507:VAL:HG23	1.98	0.46
1:B:377:PRO:HG3	1:B:443:ILE:HG13	1.98	0.46
1:D:524:PRO:HD3	1:D:905:PRO:HG3	1.98	0.46
1:E:391:ASN:HD22	1:E:418:ASN:HD22	1.64	0.46
1:A:277:LEU:HD21	1:A:610:GLN:CG	2.47	0.45
1:B:277:LEU:HD21	1:B:610:GLN:HG3	1.98	0.45
1:B:770:TRP:CE3	1:B:773:ASN:HB2	2.50	0.45
1:B:889:PRO:HD2	1:B:951:LEU:HD21	1.98	0.45
1:D:377:PRO:HB2	1:D:400:PHE:O	2.16	0.45
1:D:861:PRO:HB3	1:D:879:THR:HG21	1.98	0.45
1:E:1274:ASP:CB	1:E:1277:THR:HG22	2.41	0.45
1:F:154:VAL:HG23	1:F:170:PHE:HB3	1.97	0.45
1:F:520:LEU:HD23	1:F:757:ASP:HA	1.96	0.45
1:A:614:GLY:HA3	1:A:854:ASN:ND2	2.30	0.45
1:A:845:ILE:HG22	1:A:883:LEU:O	2.17	0.45
1:A:889:PRO:HD2	1:A:951:LEU:HD21	1.98	0.45
1:B:371:PRO:HD2	1:B:374:TRP:CD2	2.51	0.45
1:C:749:ARG:NH1	1:C:1034:PHE:O	2.49	0.45
1:D:396:THR:CG2	1:D:404:ARG:HE	2.29	0.45
1:D:570:GLN:HG2	1:D:596:GLY:CA	2.44	0.45
1:E:178:THR:O	1:E:358:VAL:HG11	2.16	0.45
1:F:277:LEU:HD21	1:F:610:GLN:HG3	1.98	0.45
1:F:841:GLN:HE22	1:F:843:ASN:HB2	1.81	0.45
1:A:115:LEU:HD11	1:A:324:LEU:HD13	1.99	0.45
1:C:524:PRO:HD3	1:C:905:PRO:HG3	1.98	0.45
1:E:1008:ASP:HB3	1:E:1061:TRP:CD1	2.52	0.45
1:F:1112:VAL:HA	1:F:1127:PRO:HA	1.99	0.45
1:B:115:LEU:HD11	1:B:324:LEU:HD13	1.98	0.45
1:B:277:LEU:HD22	1:B:620:HIS:CD2	2.51	0.45
1:D:770:TRP:CE3	1:D:773:ASN:HB2	2.51	0.45
1:D:1013:VAL:HG11	1:D:1075:PRO:HB3	1.99	0.45
1:D:377:PRO:HG3	1:D:443:ILE:HG13	1.98	0.45
1:D:466:ILE:HB	1:D:487:PHE:HB2	1.97	0.45
1:F:1269:VAL:HA	1:F:1272:LEU:HD12	1.99	0.45
1:A:448:GLU:H	1:A:448:GLU:HG2	1.46	0.45
1:B:245:PRO:HG2	1:B:568:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:VAL:HG22	1:B:293:ASN:HA	1.99	0.45
1:B:1112:VAL:HA	1:B:1127:PRO:HA	1.99	0.45
1:B:1191:SER:HB2	1:B:1196:THR:HG23	1.98	0.45
1:D:1312:GLN:O	1:D:1345:PRO:HD2	2.17	0.45
1:E:377:PRO:HG3	1:E:443:ILE:HG13	1.97	0.45
1:E:770:TRP:CE3	1:E:773:ASN:HB2	2.50	0.45
1:F:391:ASN:HD22	1:F:418:ASN:HD22	1.64	0.45
1:A:281:VAL:HG22	1:A:293:ASN:HA	1.99	0.45
1:B:504:PRO:HG2	1:B:507:VAL:HG23	1.99	0.45
1:C:275:LYS:HG3	1:C:644:TYR:HE1	1.80	0.45
1:C:1269:VAL:HA	1:C:1272:LEU:HD12	1.98	0.45
1:D:277:LEU:HD22	1:D:620:HIS:CD2	2.52	0.45
1:E:162:PRO:HG3	1:E:344:TYR:CE2	2.52	0.45
1:E:524:PRO:HD3	1:E:905:PRO:HG3	1.97	0.45
1:E:841:GLN:HE22	1:E:843:ASN:HB2	1.82	0.45
1:F:1321:LYS:HB2	1:F:1328:PHE:CE1	2.52	0.45
1:C:115:LEU:HD11	1:C:324:LEU:HD13	1.98	0.45
1:C:841:GLN:HE22	1:C:843:ASN:HB2	1.81	0.45
1:D:793:LEU:HD22	1:D:801:VAL:HG13	1.98	0.45
1:E:245:PRO:HG2	1:E:568:TYR:HB2	1.98	0.45
1:F:793:LEU:HD22	1:F:801:VAL:HG13	1.99	0.45
1:A:520:LEU:HD23	1:A:757:ASP:HA	1.99	0.45
1:C:651:LYS:HE3	1:D:823:ASN:HD21	1.82	0.45
1:D:1143:LEU:O	1:D:1149:ILE:HD11	2.17	0.45
1:E:277:LEU:HD21	1:E:610:GLN:HG3	1.98	0.45
1:F:570:GLN:HG2	1:F:596:GLY:CA	2.46	0.45
1:C:770:TRP:CE3	1:C:773:ASN:HB2	2.51	0.45
1:F:178:THR:O	1:F:358:VAL:HG11	2.16	0.45
1:F:277:LEU:HD21	1:F:610:GLN:CG	2.46	0.45
1:A:732:LEU:HD13	1:A:732:LEU:HA	1.87	0.44
1:B:467:PHE:CG	1:B:542:VAL:HG21	2.52	0.44
1:D:811:LEU:HD23	1:D:817:ARG:CZ	2.48	0.44
1:E:277:LEU:HD21	1:E:610:GLN:CG	2.46	0.44
1:E:1269:VAL:HA	1:E:1272:LEU:HD12	1.99	0.44
1:F:845:ILE:HG22	1:F:883:LEU:O	2.17	0.44
1:A:525:LEU:HD21	1:A:557:MET:HG2	1.98	0.44
1:A:749:ARG:NH1	1:A:1034:PHE:O	2.51	0.44
1:A:1003:ASN:ND2	1:A:1146:THR:HG21	2.32	0.44
1:B:628:ILE:HD12	1:B:657:ARG:HD3	1.99	0.44
1:D:162:PRO:HG3	1:D:344:TYR:CE2	2.52	0.44
1:F:373:SER:HB2	1:F:374:TRP:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:466:ILE:HB	1:F:487:PHE:HB2	1.97	0.44
1:F:1013:VAL:HG11	1:F:1075:PRO:HB3	1.99	0.44
1:A:524:PRO:HD3	1:A:905:PRO:HG3	2.00	0.44
1:A:710:ILE:HD11	1:A:712:TYR:CZ	2.52	0.44
1:A:792:PRO:HG3	1:A:967:HIS:CE1	2.53	0.44
1:A:1112:VAL:HA	1:A:1127:PRO:HA	1.98	0.44
1:B:162:PRO:HG3	1:B:344:TYR:CE2	2.53	0.44
1:C:672:LYS:NZ	1:D:814:GLU:O	2.42	0.44
1:F:165:ASP:HB3	1:F:168:LYS:HB2	1.98	0.44
1:F:238:GLN:HE21	1:F:239:ARG:HG2	1.81	0.44
1:F:1191:SER:HB2	1:F:1196:THR:HG23	1.99	0.44
1:A:177:PRO:HG2	1:A:180:TRP:CE3	2.53	0.44
1:B:177:PRO:HG2	1:B:180:TRP:CE3	2.53	0.44
1:B:710:ILE:HD11	1:B:712:TYR:CZ	2.52	0.44
1:B:1269:VAL:HA	1:B:1272:LEU:HD12	1.98	0.44
1:C:58:GLN:OE1	1:C:149:GLU:CB	2.65	0.44
1:C:1013:VAL:HG11	1:C:1075:PRO:HB3	1.99	0.44
1:D:277:LEU:HB2	1:D:653:VAL:HB	1.98	0.44
1:F:275:LYS:HG3	1:F:644:TYR:HE1	1.82	0.44
1:A:92:ARG:HG3	1:A:128:PHE:CD1	2.53	0.44
1:A:1269:VAL:HA	1:A:1272:LEU:HD12	1.99	0.44
1:A:1334:ALA:HB3	1:A:1339:PRO:HA	2.00	0.44
1:B:570:GLN:HG2	1:B:596:GLY:CA	2.46	0.44
1:B:1109:PRO:HB3	1:B:1137:MET:SD	2.57	0.44
1:C:926:SER:O	1:C:983:ILE:HG12	2.18	0.44
1:A:378:LYS:O	1:A:397:THR:HG23	2.17	0.44
1:B:749:ARG:NH1	1:B:1034:PHE:O	2.51	0.44
1:E:91:VAL:HG21	1:E:131:ARG:CZ	2.47	0.44
1:E:524:PRO:HD2	1:E:557:MET:CE	2.48	0.44
1:E:1003:ASN:ND2	1:E:1146:THR:HG21	2.32	0.44
1:F:228:LYS:NZ	1:F:1096:THR:HG21	2.31	0.44
1:F:525:LEU:HD21	1:F:557:MET:HG2	2.00	0.44
1:F:749:ARG:NH1	1:F:1034:PHE:O	2.50	0.44
1:A:651:LYS:HE3	1:B:823:ASN:HD21	1.83	0.44
1:B:1334:ALA:HB3	1:B:1339:PRO:HA	2.00	0.44
1:C:178:THR:O	1:C:358:VAL:HG11	2.18	0.44
1:C:793:LEU:HD12	1:C:941:TRP:HE3	1.82	0.44
1:C:1008:ASP:HB3	1:C:1061:TRP:CD1	2.51	0.44
1:D:749:ARG:NH1	1:D:1034:PHE:O	2.51	0.44
1:A:72:ASN:HB2	1:A:473:ALA:HB2	1.99	0.44
1:A:396:THR:CG2	1:A:404:ARG:HE	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:ASP:HB3	1:A:1061:TRP:CD1	2.52	0.44
1:B:470:ASN:OD1	1:B:472:HIS:HB2	2.18	0.44
1:B:861:PRO:HB3	1:B:879:THR:HG21	2.00	0.44
1:B:1143:LEU:O	1:B:1149:ILE:HD11	2.18	0.44
1:C:1112:VAL:HA	1:C:1127:PRO:HA	1.99	0.44
1:E:152:SER:OG	1:E:172:LEU:HB3	2.18	0.44
1:F:1292:PRO:HG2	1:F:1295:PHE:HB2	2.00	0.44
1:D:100:ILE:HD12	1:D:100:ILE:H	1.83	0.44
1:D:245:PRO:HG2	1:D:568:TYR:HB2	2.00	0.44
1:E:845:ILE:HG22	1:E:883:LEU:O	2.17	0.44
1:E:1191:SER:HB2	1:E:1196:THR:HG23	2.00	0.44
1:B:536:ARG:NH1	1:B:686:ASN:HB3	2.33	0.43
1:C:135:ASN:HD22	1:C:1330:PRO:HD2	1.83	0.43
1:D:115:LEU:HD11	1:D:324:LEU:HD13	2.00	0.43
1:D:200:LEU:HD12	1:D:344:TYR:CE2	2.53	0.43
1:D:277:LEU:HD21	1:D:610:GLN:HG3	2.00	0.43
1:D:628:ILE:HD12	1:D:657:ARG:HD3	2.00	0.43
1:F:524:PRO:HD3	1:F:905:PRO:HG3	2.00	0.43
1:F:628:ILE:HD12	1:F:657:ARG:HD3	2.00	0.43
1:F:1008:ASP:HB3	1:F:1061:TRP:CD1	2.52	0.43
1:A:238:GLN:HE21	1:A:239:ARG:HG2	1.84	0.43
1:B:559:ASP:OD2	1:B:562:THR:HB	2.18	0.43
1:D:177:PRO:HG2	1:D:180:TRP:CE3	2.53	0.43
1:D:1112:VAL:HA	1:D:1127:PRO:HA	2.00	0.43
1:D:1269:VAL:HA	1:D:1272:LEU:HD12	1.99	0.43
1:E:793:LEU:HD22	1:E:801:VAL:HG13	1.99	0.43
1:F:470:ASN:OD1	1:F:472:HIS:HB2	2.18	0.43
1:A:373:SER:HB2	1:A:374:TRP:HD1	1.83	0.43
1:A:405:HIS:HE1	1:A:686:ASN:O	2.01	0.43
1:B:237:THR:HG21	1:B:575:LEU:HD13	2.01	0.43
1:C:237:THR:HG21	1:C:575:LEU:HD13	2.00	0.43
1:C:628:ILE:HD12	1:C:657:ARG:HD3	2.00	0.43
1:D:504:PRO:HG2	1:D:507:VAL:HG23	1.99	0.43
1:D:732:LEU:HD13	1:D:732:LEU:HA	1.87	0.43
1:A:200:LEU:HD12	1:A:344:TYR:CE2	2.52	0.43
1:D:152:SER:OG	1:D:172:LEU:HB3	2.18	0.43
1:E:238:GLN:HE21	1:E:239:ARG:HG2	1.83	0.43
1:E:628:ILE:HD12	1:E:657:ARG:HD3	2.01	0.43
1:E:1112:VAL:HA	1:E:1127:PRO:HA	1.99	0.43
1:E:1261:PHE:CE1	1:E:1345:PRO:HA	2.54	0.43
1:F:115:LEU:HD11	1:F:324:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:PRO:HG2	1:F:180:TRP:CE3	2.52	0.43
1:F:1193:GLN:HE21	1:F:1193:GLN:HB3	1.59	0.43
1:B:524:PRO:HD3	1:B:905:PRO:HG3	2.00	0.43
1:B:599:ASN:HB2	1:B:658:TYR:O	2.18	0.43
1:B:987:ALA:CA	1:B:1115:TYR:CD2	3.02	0.43
1:C:72:ASN:HB2	1:C:473:ALA:HB2	2.01	0.43
1:C:1003:ASN:ND2	1:C:1146:THR:HG21	2.32	0.43
1:E:467:PHE:CG	1:E:542:VAL:HG21	2.54	0.43
1:F:327:THR:HG21	1:F:367:VAL:HG21	1.99	0.43
1:F:770:TRP:CE3	1:F:773:ASN:HB2	2.51	0.43
1:A:793:LEU:HD12	1:A:941:TRP:HE3	1.83	0.43
1:B:92:ARG:HG3	1:B:128:PHE:CE1	2.54	0.43
1:C:271:SER:HB2	1:C:868:VAL:HG22	2.01	0.43
1:C:373:SER:HB2	1:C:374:TRP:HD1	1.82	0.43
1:D:72:ASN:HB2	1:D:473:ALA:HB2	2.00	0.43
1:D:237:THR:HG21	1:D:575:LEU:HD13	2.01	0.43
1:F:945:GLU:H	1:F:945:GLU:HG3	1.24	0.43
1:A:699:ASN:ND2	1:A:702:LEU:HB2	2.34	0.43
1:B:793:LEU:HD12	1:B:941:TRP:HE3	1.83	0.43
1:C:1334:ALA:HB3	1:C:1339:PRO:HA	2.01	0.43
1:E:1301:ARG:HG2	1:E:1328:PHE:CD2	2.54	0.43
1:F:91:VAL:HG21	1:F:131:ARG:CZ	2.48	0.43
1:F:374:TRP:CD1	1:F:374:TRP:N	2.87	0.43
1:F:1321:LYS:HA	1:F:1328:PHE:CD1	2.53	0.43
1:C:1041:TYR:CE1	1:C:1181:ASN:HB2	2.54	0.43
1:A:467:PHE:CG	1:A:542:VAL:HG21	2.54	0.43
1:A:470:ASN:OD1	1:A:472:HIS:HB2	2.19	0.43
1:C:396:THR:CG2	1:C:404:ARG:HE	2.31	0.43
1:C:599:ASN:HB2	1:C:658:TYR:O	2.19	0.43
1:D:165:ASP:HB3	1:D:168:LYS:HB2	2.01	0.43
1:D:273:ARG:HD3	1:D:619:PRO:HB3	2.01	0.43
1:D:1097:ASN:HB2	1:D:1098:PRO:CD	2.43	0.43
1:A:1191:SER:HB2	1:A:1196:THR:HG23	2.00	0.43
1:B:277:LEU:HD22	1:B:620:HIS:HD2	1.84	0.43
1:B:1003:ASN:ND2	1:B:1146:THR:HG21	2.33	0.43
1:C:277:LEU:HD21	1:C:610:GLN:CG	2.49	0.43
1:C:277:LEU:HD21	1:C:610:GLN:HG3	2.00	0.43
1:E:165:ASP:HB3	1:E:168:LYS:HB2	2.01	0.43
1:E:200:LEU:HD12	1:E:344:TYR:CE2	2.53	0.43
1:E:396:THR:CG2	1:E:404:ARG:HE	2.32	0.43
1:E:570:GLN:HG2	1:E:596:GLY:CA	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PRO:HG3	1:A:344:TYR:CE2	2.54	0.42
1:B:273:ARG:HD3	1:B:619:PRO:HB3	2.01	0.42
1:B:396:THR:CG2	1:B:404:ARG:HE	2.31	0.42
1:B:793:LEU:HD22	1:B:801:VAL:HG13	2.01	0.42
1:B:913:ARG:NH2	1:B:920:PRO:HD3	2.34	0.42
1:B:1008:ASP:HB3	1:B:1061:TRP:CD1	2.54	0.42
1:C:172:LEU:HD11	1:C:351:ASN:HB3	2.01	0.42
1:C:504:PRO:HG2	1:C:507:VAL:HG23	2.01	0.42
1:C:811:LEU:HD21	1:C:895:ASN:O	2.19	0.42
1:C:1070:ASP:HB3	1:C:1072:ASP:OD1	2.19	0.42
1:D:811:LEU:HD23	1:D:817:ARG:NE	2.34	0.42
1:E:72:ASN:HB2	1:E:473:ALA:HB2	2.01	0.42
1:E:281:VAL:HG22	1:E:293:ASN:HA	2.00	0.42
1:A:861:PRO:HB3	1:A:879:THR:HG21	2.01	0.42
1:A:913:ARG:NH2	1:A:920:PRO:HD3	2.34	0.42
1:B:148:MET:HE1	1:B:355:PHE:HZ	1.84	0.42
1:C:228:LYS:NZ	1:C:239:ARG:HH12	2.17	0.42
1:C:983:ILE:HD11	1:C:1152:LYS:HD2	2.00	0.42
1:D:92:ARG:HG3	1:D:128:PHE:CD1	2.54	0.42
1:D:194:SER:CB	1:D:200:LEU:HD23	2.48	0.42
1:D:1191:SER:HB2	1:D:1196:THR:HG23	2.00	0.42
1:F:152:SER:OG	1:F:172:LEU:HB3	2.18	0.42
1:F:467:PHE:CG	1:F:542:VAL:HG21	2.54	0.42
1:A:1319:GLU:HB3	1:A:1328:PHE:HB3	2.00	0.42
1:B:525:LEU:HD21	1:B:557:MET:HG2	2.00	0.42
1:C:59:GLN:HB2	1:C:143:ILE:H	1.84	0.42
1:D:178:THR:O	1:D:358:VAL:HG11	2.19	0.42
1:D:1319:GLU:HB3	1:D:1328:PHE:HB3	2.01	0.42
1:E:373:SER:HB2	1:E:374:TRP:HD1	1.84	0.42
1:E:1292:PRO:HG2	1:E:1295:PHE:HB2	2.00	0.42
1:F:281:VAL:HG22	1:F:293:ASN:HA	2.00	0.42
1:F:396:THR:CG2	1:F:404:ARG:HE	2.31	0.42
1:F:994:SER:HB2	1:F:1137:MET:HE2	2.01	0.42
1:A:1070:ASP:HB3	1:A:1072:ASP:OD1	2.20	0.42
1:B:792:PRO:HG3	1:B:967:HIS:CE1	2.54	0.42
1:C:448:GLU:H	1:C:448:GLU:HG2	1.48	0.42
1:C:651:LYS:CE	1:D:823:ASN:HD21	2.32	0.42
1:D:405:HIS:HE1	1:D:686:ASN:O	2.02	0.42
1:D:811:LEU:HD11	1:D:895:ASN:OD1	2.20	0.42
1:D:841:GLN:HE22	1:D:843:ASN:HB2	1.85	0.42
1:E:470:ASN:OD1	1:E:472:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:749:ARG:NH1	1:E:1034:PHE:O	2.52	0.42
1:A:244:SER:HA	1:A:571:LEU:HD22	2.01	0.42
1:A:628:ILE:HD12	1:A:657:ARG:HD3	2.00	0.42
1:B:72:ASN:HB2	1:B:473:ALA:HB2	2.00	0.42
1:B:165:ASP:HB3	1:B:168:LYS:HB2	2.02	0.42
1:D:92:ARG:HG3	1:D:128:PHE:CE1	2.55	0.42
1:D:467:PHE:CG	1:D:542:VAL:HG21	2.54	0.42
1:D:1334:ALA:HB3	1:D:1339:PRO:HA	2.01	0.42
1:F:201:TYR:CE1	1:F:345:ASP:HB3	2.55	0.42
1:F:1274:ASP:CB	1:F:1277:THR:HG22	2.40	0.42
1:A:165:ASP:HB3	1:A:168:LYS:HB2	2.02	0.42
1:B:1261:PHE:CE1	1:B:1345:PRO:HA	2.52	0.42
1:C:177:PRO:HG2	1:C:180:TRP:CE3	2.54	0.42
1:C:817:ARG:NE	1:C:817:ARG:HA	2.34	0.42
1:D:994:SER:HB2	1:D:1137:MET:HE3	2.02	0.42
1:D:1070:ASP:HB3	1:D:1072:ASP:OD1	2.19	0.42
1:E:1013:VAL:HG11	1:E:1075:PRO:HB3	2.02	0.42
1:F:1301:ARG:CG	1:F:1328:PHE:HE2	2.32	0.42
1:A:749:ARG:HG3	1:A:749:ARG:HH21	1.84	0.42
1:A:817:ARG:NE	1:A:817:ARG:HA	2.35	0.42
1:A:841:GLN:HE22	1:A:843:ASN:HB2	1.84	0.42
1:B:405:HIS:HE1	1:B:686:ASN:O	2.03	0.42
1:D:710:ILE:HD11	1:D:712:TYR:CZ	2.54	0.42
1:E:994:SER:HB2	1:E:1137:MET:HE3	2.02	0.42
1:F:72:ASN:HB2	1:F:473:ALA:HB2	2.02	0.42
1:F:536:ARG:NH1	1:F:686:ASN:HB3	2.35	0.42
1:F:1003:ASN:ND2	1:F:1146:THR:HG21	2.33	0.42
1:A:1189:GLU:OE2	1:B:729:LEU:HD11	2.20	0.42
1:B:152:SER:OG	1:B:172:LEU:HB3	2.20	0.42
1:B:732:LEU:HD13	1:B:732:LEU:HA	1.90	0.42
1:B:987:ALA:HA	1:B:1115:TYR:CD2	2.55	0.42
1:C:244:SER:HA	1:C:571:LEU:HD22	2.02	0.42
1:C:536:ARG:NH1	1:C:686:ASN:HB3	2.34	0.42
1:D:122:LEU:HB3	1:D:126:GLN:NE2	2.35	0.42
1:D:617:PHE:CE2	1:D:859:PHE:HB2	2.54	0.42
1:D:773:ASN:HB3	1:D:775:LYS:HB2	2.01	0.42
1:E:543:LYS:HD2	1:E:1012:LEU:HB3	2.02	0.42
1:E:557:MET:HE2	1:E:557:MET:HB3	1.85	0.42
1:E:1097:ASN:HB3	1:E:1098:PRO:HD3	2.02	0.42
1:F:543:LYS:HD2	1:F:1012:LEU:HB3	2.02	0.42
1:F:599:ASN:HB2	1:F:658:TYR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:GLN:O	1:A:1345:PRO:HD2	2.20	0.42
1:B:587:GLU:HG3	1:B:1107:TYR:HE1	1.85	0.42
1:B:1070:ASP:HB3	1:B:1072:ASP:OD1	2.19	0.42
1:C:152:SER:OG	1:C:172:LEU:HB3	2.20	0.42
1:D:1003:ASN:ND2	1:D:1146:THR:HG21	2.34	0.42
1:E:115:LEU:HD11	1:E:324:LEU:HD13	2.01	0.42
1:A:1141:LEU:HD12	1:A:1141:LEU:HA	1.93	0.42
1:B:92:ARG:HG3	1:B:128:PHE:CD1	2.54	0.42
1:B:374:TRP:N	1:B:374:TRP:CD1	2.87	0.42
1:B:1319:GLU:HB3	1:B:1328:PHE:HB3	2.01	0.42
1:C:467:PHE:CG	1:C:542:VAL:HG21	2.55	0.42
1:C:470:ASN:OD1	1:C:472:HIS:HB2	2.18	0.42
1:C:994:SER:HB2	1:C:1137:MET:HE3	2.01	0.42
1:E:92:ARG:HG3	1:E:128:PHE:CE2	2.54	0.42
1:E:509:PHE:HZ	1:E:537:MET:HE1	1.84	0.42
1:F:237:THR:HG21	1:F:575:LEU:HD13	2.02	0.42
1:F:793:LEU:HD12	1:F:941:TRP:HE3	1.85	0.42
1:F:983:ILE:HD11	1:F:1152:LYS:HD2	2.02	0.42
1:A:1097:ASN:HB3	1:A:1098:PRO:HD2	1.99	0.41
1:B:238:GLN:HE21	1:B:239:ARG:HG2	1.85	0.41
1:C:661:LEU:HD13	1:C:901:ASN:HD21	1.85	0.41
1:D:536:ARG:NH1	1:D:686:ASN:HB3	2.35	0.41
1:D:923:ILE:HD13	1:D:923:ILE:HA	1.85	0.41
1:E:109:ASP:HB3	1:E:113:LYS:HD3	2.02	0.41
1:F:543:LYS:HB2	1:F:1012:LEU:HD13	2.02	0.41
1:C:391:ASN:ND2	1:C:418:ASN:HD22	2.18	0.41
1:C:850:VAL:CG2	1:C:851:LYS:N	2.83	0.41
1:D:599:ASN:HB2	1:D:658:TYR:O	2.20	0.41
1:D:631:ASN:OD1	1:D:633:ASN:HB2	2.20	0.41
1:A:1279:PHE:HE1	1:A:1301:ARG:HD2	1.72	0.41
1:B:244:SER:HA	1:B:571:LEU:HD22	2.03	0.41
1:B:888:SER:HB2	1:B:889:PRO:HD2	2.02	0.41
1:B:1013:VAL:HG11	1:B:1075:PRO:HB3	2.02	0.41
1:C:162:PRO:HG3	1:C:344:TYR:CE2	2.54	0.41
1:C:164:PHE:CZ	1:C:166:PRO:HA	2.55	0.41
1:C:810:HIS:CE1	1:C:814:GLU:HG2	2.54	0.41
1:E:172:LEU:HD11	1:E:351:ASN:HB3	2.03	0.41
1:E:374:TRP:N	1:E:374:TRP:CD1	2.87	0.41
1:F:509:PHE:HZ	1:F:537:MET:HE1	1.85	0.41
1:B:696:ALA:HB1	1:B:747:VAL:HG12	2.01	0.41
1:C:200:LEU:HD12	1:C:344:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:939:GLN:HE21	1:C:950:ASN:HB2	1.84	0.41
1:D:100:ILE:CD1	1:D:100:ILE:H	2.33	0.41
1:D:924:ASN:CB	1:D:985:PHE:HA	2.51	0.41
1:D:945:GLU:H	1:D:945:GLU:HG3	1.25	0.41
1:E:983:ILE:HD11	1:E:1152:LYS:HD2	2.03	0.41
1:A:237:THR:HG21	1:A:575:LEU:HD13	2.01	0.41
1:A:1137:MET:HE2	1:A:1137:MET:HB2	1.57	0.41
1:B:194:SER:CB	1:B:200:LEU:HD23	2.49	0.41
1:B:923:ILE:HD13	1:B:923:ILE:HA	1.87	0.41
1:C:122:LEU:HB3	1:C:126:GLN:NE2	2.33	0.41
1:E:237:THR:HG21	1:E:575:LEU:HD13	2.02	0.41
1:E:710:ILE:HD11	1:E:712:TYR:CZ	2.55	0.41
1:F:835:ARG:HB3	1:F:1122:ASN:HA	2.02	0.41
1:A:135:ASN:HD22	1:A:1330:PRO:HD2	1.86	0.41
1:A:599:ASN:HB2	1:A:658:TYR:O	2.20	0.41
1:B:810:HIS:ND1	1:B:817:ARG:HD3	2.35	0.41
1:C:631:ASN:OD1	1:C:633:ASN:HB2	2.20	0.41
1:C:846:PRO:HG2	1:C:849:GLN:NE2	2.36	0.41
1:C:1312:GLN:O	1:C:1345:PRO:HD2	2.21	0.41
1:C:1319:GLU:HB3	1:C:1328:PHE:HB3	2.01	0.41
1:D:846:PRO:HG2	1:D:849:GLN:NE2	2.35	0.41
1:F:135:ASN:HD22	1:F:1330:PRO:HD2	1.84	0.41
1:F:1097:ASN:HB3	1:F:1098:PRO:HD3	2.03	0.41
1:A:164:PHE:CZ	1:A:166:PRO:HA	2.55	0.41
1:B:845:ILE:HG22	1:B:883:LEU:O	2.21	0.41
1:B:1301:ARG:HG2	1:B:1328:PHE:CD2	2.56	0.41
1:C:91:VAL:HG21	1:C:131:ARG:CZ	2.51	0.41
1:C:525:LEU:HD21	1:C:557:MET:HG2	2.03	0.41
1:C:861:PRO:HB3	1:C:879:THR:HG21	2.03	0.41
1:D:135:ASN:HD22	1:D:1330:PRO:HD2	1.85	0.41
1:E:271:SER:HB2	1:E:868:VAL:HG22	2.02	0.41
1:E:1036:ARG:HH21	1:F:742:ARG:NH1	2.19	0.41
1:E:1312:GLN:O	1:E:1345:PRO:HD2	2.19	0.41
1:A:850:VAL:CG2	1:A:851:LYS:N	2.84	0.41
1:B:99:ASN:ND2	1:B:102:SER:HB3	2.35	0.41
1:B:122:LEU:HB3	1:B:126:GLN:NE2	2.35	0.41
1:B:467:PHE:CD1	1:B:542:VAL:HG21	2.56	0.41
1:C:374:TRP:N	1:C:374:TRP:CD1	2.88	0.41
1:C:702:LEU:HD12	1:C:702:LEU:HA	1.87	0.41
1:D:696:ALA:HB1	1:D:747:VAL:HG12	2.02	0.41
1:F:527:THR:HB	1:F:533:TYR:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HB3	1:A:126:GLN:NE2	2.34	0.41
1:A:243:ASP:HB2	1:A:309:VAL:HG11	2.03	0.41
1:A:271:SER:HB2	1:A:868:VAL:HG22	2.03	0.41
1:B:543:LYS:HD2	1:B:1012:LEU:HB3	2.03	0.41
1:B:615:SER:N	1:B:854:ASN:HD21	2.18	0.41
1:B:749:ARG:HH21	1:B:749:ARG:HG3	1.85	0.41
1:B:809:GLN:HB2	1:B:828:ILE:CD1	2.50	0.41
1:B:939:GLN:HE21	1:B:950:ASN:HB2	1.85	0.41
1:C:405:HIS:HE1	1:C:686:ASN:O	2.03	0.41
1:C:587:GLU:HG3	1:C:1107:TYR:HE1	1.86	0.41
1:C:835:ARG:HB3	1:C:1122:ASN:HA	2.02	0.41
1:C:926:SER:O	1:C:983:ILE:HG23	2.20	0.41
1:C:1261:PHE:CE1	1:C:1345:PRO:HA	2.56	0.41
1:D:1032:THR:OG1	1:D:1043:GLY:HA2	2.20	0.41
1:E:92:ARG:HG3	1:E:128:PHE:CD2	2.56	0.41
1:E:661:LEU:HD13	1:E:901:ASN:HD21	1.85	0.41
1:E:1334:ALA:HB3	1:E:1339:PRO:HA	2.02	0.41
1:F:92:ARG:HG3	1:F:128:PHE:CE2	2.55	0.41
1:F:122:LEU:HB3	1:F:126:GLN:NE2	2.36	0.41
1:F:1248:THR:HA	1:F:1251:ILE:HD12	2.03	0.41
1:F:1319:GLU:HB3	1:F:1328:PHE:HB3	2.02	0.41
1:F:1321:LYS:HA	1:F:1328:PHE:HD1	1.86	0.41
1:A:172:LEU:HD11	1:A:351:ASN:HB3	2.03	0.41
1:A:696:ALA:HB1	1:A:747:VAL:HG12	2.03	0.41
1:B:987:ALA:CA	1:B:1115:TYR:HD2	2.34	0.41
1:C:543:LYS:HB2	1:C:1012:LEU:HD13	2.03	0.41
1:D:201:TYR:CE1	1:D:345:ASP:HB3	2.56	0.41
1:D:244:SER:HA	1:D:571:LEU:HD22	2.03	0.41
1:E:702:LEU:HD12	1:E:702:LEU:HA	1.92	0.41
1:E:793:LEU:HD12	1:E:941:TRP:HE3	1.86	0.41
1:E:945:GLU:H	1:E:945:GLU:HG3	1.24	0.41
1:E:1319:GLU:HB3	1:E:1328:PHE:HB3	2.02	0.41
1:F:244:SER:HA	1:F:571:LEU:HD22	2.03	0.41
1:A:130:ILE:HG13	1:A:143:ILE:HG23	2.03	0.40
1:A:543:LYS:HD2	1:A:1012:LEU:HB3	2.03	0.40
1:A:661:LEU:HD13	1:A:901:ASN:HD21	1.86	0.40
1:B:773:ASN:HB3	1:B:775:LYS:HB2	2.03	0.40
1:B:983:ILE:HD11	1:B:1152:LYS:HD2	2.01	0.40
1:C:792:PRO:HG3	1:C:967:HIS:CE1	2.56	0.40
1:D:115:LEU:HD23	1:D:115:LEU:HA	1.88	0.40
1:D:391:ASN:ND2	1:D:418:ASN:HD22	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:ARG:HD3	1:F:619:PRO:HB3	2.03	0.40
1:A:91:VAL:HG21	1:A:131:ARG:CZ	2.52	0.40
1:A:397:THR:HG22	1:A:418:ASN:OD1	2.21	0.40
1:A:579:ALA:HA	1:A:582:GLN:HB2	2.04	0.40
1:A:923:ILE:HD13	1:A:923:ILE:HA	1.87	0.40
1:B:527:THR:HB	1:B:533:TYR:HB3	2.02	0.40
1:C:682:PHE:HE2	1:D:820:PHE:CE1	2.40	0.40
1:C:1031:PHE:CE1	1:C:1044:ILE:HD11	2.56	0.40
1:D:809:GLN:NE2	1:D:828:ILE:HD12	2.36	0.40
1:D:888:SER:HB2	1:D:889:PRO:HD2	2.04	0.40
1:E:1141:LEU:HD12	1:E:1141:LEU:HA	1.95	0.40
1:A:109:ASP:HB3	1:A:113:LYS:HD2	2.00	0.40
1:A:467:PHE:CD1	1:A:542:VAL:HG21	2.55	0.40
1:A:823:ASN:HD21	1:B:651:LYS:HE3	1.86	0.40
1:B:631:ASN:OD1	1:B:633:ASN:HB2	2.22	0.40
1:C:151:PRO:HG3	1:C:180:TRP:CE2	2.57	0.40
1:D:527:THR:HB	1:D:533:TYR:HB3	2.03	0.40
1:D:570:GLN:HG3	1:D:573:LYS:HE2	2.03	0.40
1:D:792:PRO:HG3	1:D:967:HIS:CE1	2.56	0.40
1:D:811:LEU:HD13	1:D:894:ILE:CG1	2.51	0.40
1:D:983:ILE:HD11	1:D:1152:LYS:HD2	2.03	0.40
1:D:1301:ARG:HG2	1:D:1328:PHE:CD2	2.56	0.40
1:E:123:ASP:OD1	1:E:208:LYS:HE2	2.20	0.40
1:E:536:ARG:NH1	1:E:686:ASN:HB3	2.36	0.40
1:E:599:ASN:HB2	1:E:658:TYR:O	2.20	0.40
1:E:835:ARG:HB3	1:E:1122:ASN:HA	2.02	0.40
1:F:231:GLN:HG3	1:F:1096:THR:HA	2.02	0.40
1:F:1318:LEU:HB3	1:F:1331:VAL:HB	2.03	0.40
1:A:374:TRP:CD1	1:A:374:TRP:N	2.86	0.40
1:A:536:ARG:NH1	1:A:686:ASN:HB3	2.36	0.40
1:B:835:ARG:HB3	1:B:1122:ASN:HA	2.03	0.40
1:D:661:LEU:HD13	1:D:901:ASN:HD21	1.85	0.40
1:D:702:LEU:HD12	1:D:702:LEU:HA	1.87	0.40
1:D:749:ARG:HH21	1:D:749:ARG:HG3	1.86	0.40
1:E:939:GLN:HE21	1:E:950:ASN:HB2	1.87	0.40
1:F:200:LEU:HD12	1:F:344:TYR:CE2	2.55	0.40
1:F:661:LEU:HD13	1:F:901:ASN:HD21	1.85	0.40
1:A:817:ARG:HG2	1:A:817:ARG:NH2	2.35	0.40
1:B:661:LEU:HD13	1:B:901:ASN:HD21	1.87	0.40
1:D:467:PHE:CD1	1:D:542:VAL:HG21	2.56	0.40
1:D:579:ALA:HA	1:D:582:GLN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:559:ASP:OD2	1:E:562:THR:HB	2.22	0.40
1:F:710:ILE:HD11	1:F:712:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1270/1304 (97%)	1128 (89%)	122 (10%)	20 (2%)	9	40
1	B	1267/1304 (97%)	1136 (90%)	114 (9%)	17 (1%)	12	44
1	C	1266/1304 (97%)	1128 (89%)	123 (10%)	15 (1%)	13	46
1	D	1263/1304 (97%)	1127 (89%)	117 (9%)	19 (2%)	10	41
1	E	1252/1304 (96%)	1118 (89%)	117 (9%)	17 (1%)	11	43
1	F	1252/1304 (96%)	1114 (89%)	119 (10%)	19 (2%)	10	41
All	All	7570/7824 (97%)	6751 (89%)	712 (9%)	107 (1%)	11	43

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	SER
1	A	1094	TYR
1	A	1097	ASN
1	A	1241	GLY
1	B	811	LEU
1	B	926	SER
1	B	1241	GLY
1	C	926	SER
1	C	1240	GLN
1	D	874	SER

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Mol	Chain	Res	Type
1	D	926	SER
1	D	1096	THR
1	D	1097	ASN
1	D	1175	THR
1	D	1240	GLN
1	E	926	SER
1	E	1241	GLY
1	F	111	ASN
1	F	926	SER
1	F	1241	GLY
1	A	99	ASN
1	A	618	GLY
1	A	827	ASP
1	A	926	SER
1	A	1057	ALA
1	A	1096	THR
1	A	1346	PHE
1	B	618	GLY
1	B	854	ASN
1	B	1057	ALA
1	C	143	ILE
1	C	618	GLY
1	C	827	ASP
1	C	1057	ALA
1	D	618	GLY
1	D	807	ILE
1	D	1057	ALA
1	E	618	GLY
1	E	874	SER
1	E	875	SER
1	E	1057	ALA
1	E	1096	THR
1	E	1346	PHE
1	F	108	SER
1	F	618	GLY
1	F	874	SER
1	F	875	SER
1	F	1057	ALA
1	F	1096	THR
1	F	1346	PHE
1	A	662	TYR
1	A	927	GLY

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Mol	Chain	Res	Type
1	A	1133	ALA
1	B	662	TYR
1	C	662	TYR
1	C	927	GLY
1	C	1094	TYR
1	C	1346	PHE
1	D	662	TYR
1	D	808	THR
1	D	1090	SER
1	E	662	TYR
1	F	662	TYR
1	A	823	ASN
1	B	143	ILE
1	B	808	THR
1	B	823	ASN
1	B	1133	ALA
1	C	1133	ALA
1	D	143	ILE
1	D	823	ASN
1	E	143	ILE
1	E	1097	ASN
1	E	1133	ALA
1	F	143	ILE
1	F	1092	THR
1	F	1097	ASN
1	F	1133	ALA
1	A	232	SER
1	B	568	TYR
1	B	1089	ASN
1	C	568	TYR
1	C	809	GLN
1	C	823	ASN
1	D	568	TYR
1	D	813	LYS
1	D	1133	ALA
1	E	568	TYR
1	E	823	ASN
1	E	1092	THR
1	F	568	TYR
1	F	823	ASN
1	A	816	THR
1	A	852	PRO

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Mol	Chain	Res	Type
1	B	227	VAL
1	B	790	SER
1	B	1094	TYR
1	C	852	PRO
1	A	1268	PRO
1	B	852	PRO
1	D	852	PRO
1	E	852	PRO
1	E	1268	PRO
1	F	852	PRO
1	F	1268	PRO
1	A	143	ILE
1	D	1268	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	1121/1146 (98%)	964 (86%)	157 (14%)	3	15
1	B	1120/1146 (98%)	965 (86%)	155 (14%)	3	15
1	C	1118/1146 (98%)	973 (87%)	145 (13%)	4	18
1	D	1117/1146 (98%)	969 (87%)	148 (13%)	4	17
1	E	1107/1146 (97%)	958 (86%)	149 (14%)	4	16
1	F	1108/1146 (97%)	958 (86%)	150 (14%)	4	16
All	All	6691/6876 (97%)	5787 (86%)	904 (14%)	4	16

All (904) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	88	PHE
1	A	91	VAL
1	A	98	LEU
1	A	101	SER

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Mol	Chain	Res	Type
1	A	106	ASN
1	A	119	GLU
1	A	125	GLN
1	A	127	ASN
1	A	130	ILE
1	A	142	ASP
1	A	143	ILE
1	A	156	ARG
1	A	158	LEU
1	A	178	THR
1	A	184	LYS
1	A	187	VAL
1	A	197	SER
1	A	203	VAL
1	A	204	LEU
1	A	218	ASN
1	A	220	VAL
1	A	222	LYS
1	A	223	GLU
1	A	225	LEU
1	A	228	LYS
1	A	235	ASN
1	A	238	GLN
1	A	239	ARG
1	A	242	LYS
1	A	251	LYS
1	A	257	SER
1	A	259	THR
1	A	268	MET
1	A	272	THR
1	A	300	LEU
1	A	301	LYS
1	A	315	LYS
1	A	324	LEU
1	A	333	GLU
1	A	334	LYS
1	A	342	SER
1	A	350	GLU
1	A	353	THR
1	A	358	VAL
1	A	373	SER
1	A	376	THR

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Mol	Chain	Res	Type
1	A	380	ASN
1	A	384	ILE
1	A	393	LEU
1	A	396	THR
1	A	404	ARG
1	A	405	HIS
1	A	415	LYS
1	A	425	VAL
1	A	431	LYS
1	A	436	LYS
1	A	437	LYS
1	A	453	ASN
1	A	458	VAL
1	A	492	THR
1	A	508	LEU
1	A	513	ILE
1	A	523	LEU
1	A	529	ARG
1	A	530	TRP
1	A	567	LYS
1	A	569	ASP
1	A	573	LYS
1	A	609	LEU
1	A	633	ASN
1	A	642	SER
1	A	649	LYS
1	A	662	TYR
1	A	685	GLU
1	A	707	SER
1	A	709	LYS
1	A	710	ILE
1	A	714	LYS
1	A	725	ARG
1	A	732	LEU
1	A	735	ASN
1	A	742	ARG
1	A	747	VAL
1	A	756	LEU
1	A	771	ILE
1	A	775	LYS
1	A	790	SER
1	A	804	LYS

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Mol	Chain	Res	Type
1	A	807	ILE
1	A	808	THR
1	A	810	HIS
1	A	814	GLU
1	A	828	ILE
1	A	835	ARG
1	A	840	ASN
1	A	841	GLN
1	A	842	LYS
1	A	853	SER
1	A	869	THR
1	A	871	SER
1	A	874	SER
1	A	883	LEU
1	A	887	ILE
1	A	908	ASN
1	A	923	ILE
1	A	929	SER
1	A	943	LYS
1	A	944	THR
1	A	945	GLU
1	A	965	LEU
1	A	974	THR
1	A	986	LYS
1	A	989	SER
1	A	993	SER
1	A	1002	LEU
1	A	1012	LEU
1	A	1030	THR
1	A	1033	ASP
1	A	1038	ARG
1	A	1039	THR
1	A	1042	LEU
1	A	1061	TRP
1	A	1067	SER
1	A	1089	ASN
1	A	1094	TYR
1	A	1106	LEU
1	A	1108	GLN
1	A	1117	THR
1	A	1120	THR
1	A	1141	LEU

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Mol	Chain	Res	Type
1	A	1150	LYS
1	A	1188	GLU
1	A	1192	ILE
1	A	1215	ASP
1	A	1220	LYS
1	A	1221	MET
1	A	1226	THR
1	A	1244	SER
1	A	1246	SER
1	A	1260	ASP
1	A	1263	ARG
1	A	1267	LEU
1	A	1270	THR
1	A	1276	ASN
1	A	1282	ASP
1	A	1287	LEU
1	A	1300	ILE
1	A	1310	GLU
1	A	1314	LEU
1	A	1318	LEU
1	A	1326	GLN
1	A	1327	GLN
1	A	1336	SER
1	A	1340	GLN
1	A	1342	VAL
1	A	1346	PHE
1	B	57	HIS
1	B	78	LEU
1	B	88	PHE
1	B	91	VAL
1	B	94	GLN
1	B	97	ASN
1	B	99	ASN
1	B	101	SER
1	B	105	LYS
1	B	108	SER
1	B	111	ASN
1	B	119	GLU
1	B	127	ASN
1	B	130	ILE
1	B	142	ASP
1	B	143	ILE

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Mol	Chain	Res	Type
1	B	149	GLU
1	B	156	ARG
1	B	158	LEU
1	B	178	THR
1	B	184	LYS
1	B	187	VAL
1	B	197	SER
1	B	203	VAL
1	B	204	LEU
1	B	218	ASN
1	B	220	VAL
1	B	222	LYS
1	B	223	GLU
1	B	225	LEU
1	B	235	ASN
1	B	238	GLN
1	B	239	ARG
1	B	242	LYS
1	B	251	LYS
1	B	257	SER
1	B	259	THR
1	B	268	MET
1	B	272	THR
1	B	300	LEU
1	B	301	LYS
1	B	315	LYS
1	B	319	GLU
1	B	324	LEU
1	B	333	GLU
1	B	334	LYS
1	B	342	SER
1	B	350	GLU
1	B	353	THR
1	B	358	VAL
1	B	372	PRO
1	B	373	SER
1	B	376	THR
1	B	380	ASN
1	B	384	ILE
1	B	393	LEU
1	B	396	THR
1	B	404	ARG

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Mol	Chain	Res	Type
1	B	405	HIS
1	B	415	LYS
1	B	431	LYS
1	B	436	LYS
1	B	437	LYS
1	B	453	ASN
1	B	492	THR
1	B	508	LEU
1	B	513	ILE
1	B	523	LEU
1	B	529	ARG
1	B	530	TRP
1	B	567	LYS
1	B	569	ASP
1	B	573	LYS
1	B	609	LEU
1	B	613	MET
1	B	633	ASN
1	B	642	SER
1	B	649	LYS
1	B	662	TYR
1	B	685	GLU
1	B	707	SER
1	B	709	LYS
1	B	710	ILE
1	B	725	ARG
1	B	732	LEU
1	B	735	ASN
1	B	747	VAL
1	B	756	LEU
1	B	771	ILE
1	B	775	LYS
1	B	804	LYS
1	B	806	MET
1	B	807	ILE
1	B	811	LEU
1	B	817	ARG
1	B	828	ILE
1	B	835	ARG
1	B	840	ASN
1	B	841	GLN
1	B	842	LYS

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Mol	Chain	Res	Type
1	B	854	ASN
1	B	883	LEU
1	B	887	ILE
1	B	908	ASN
1	B	943	LYS
1	B	944	THR
1	B	945	GLU
1	B	965	LEU
1	B	974	THR
1	B	986	LYS
1	B	989	SER
1	B	993	SER
1	B	1012	LEU
1	B	1038	ARG
1	B	1039	THR
1	B	1042	LEU
1	B	1061	TRP
1	B	1067	SER
1	B	1091	SER
1	B	1092	THR
1	B	1094	TYR
1	B	1096	THR
1	B	1106	LEU
1	B	1108	GLN
1	B	1117	THR
1	B	1120	THR
1	B	1141	LEU
1	B	1150	LYS
1	B	1192	ILE
1	B	1215	ASP
1	B	1220	LYS
1	B	1221	MET
1	B	1226	THR
1	B	1244	SER
1	B	1246	SER
1	B	1260	ASP
1	B	1263	ARG
1	B	1267	LEU
1	B	1270	THR
1	B	1276	ASN
1	B	1282	ASP
1	B	1283	GLN

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Mol	Chain	Res	Type
1	B	1287	LEU
1	B	1300	ILE
1	B	1310	GLU
1	B	1311	ASN
1	B	1314	LEU
1	B	1318	LEU
1	B	1326	GLN
1	B	1327	GLN
1	B	1336	SER
1	B	1340	GLN
1	B	1341	THR
1	B	1342	VAL
1	B	1346	PHE
1	C	58	GLN
1	C	88	PHE
1	C	91	VAL
1	C	94	GLN
1	C	99	ASN
1	C	101	SER
1	C	106	ASN
1	C	119	GLU
1	C	127	ASN
1	C	130	ILE
1	C	142	ASP
1	C	156	ARG
1	C	158	LEU
1	C	178	THR
1	C	184	LYS
1	C	187	VAL
1	C	197	SER
1	C	203	VAL
1	C	204	LEU
1	C	218	ASN
1	C	220	VAL
1	C	223	GLU
1	C	225	LEU
1	C	235	ASN
1	C	238	GLN
1	C	242	LYS
1	C	251	LYS
1	C	257	SER
1	C	259	THR

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Mol	Chain	Res	Type
1	C	272	THR
1	C	275	LYS
1	C	300	LEU
1	C	301	LYS
1	C	315	LYS
1	C	324	LEU
1	C	332	ARG
1	C	333	GLU
1	C	334	LYS
1	C	342	SER
1	C	350	GLU
1	C	353	THR
1	C	358	VAL
1	C	373	SER
1	C	376	THR
1	C	380	ASN
1	C	384	ILE
1	C	393	LEU
1	C	396	THR
1	C	404	ARG
1	C	405	HIS
1	C	415	LYS
1	C	431	LYS
1	C	436	LYS
1	C	437	LYS
1	C	453	ASN
1	C	458	VAL
1	C	492	THR
1	C	508	LEU
1	C	513	ILE
1	C	523	LEU
1	C	529	ARG
1	C	530	TRP
1	C	562	THR
1	C	567	LYS
1	C	569	ASP
1	C	573	LYS
1	C	609	LEU
1	C	633	ASN
1	C	642	SER
1	C	649	LYS
1	C	662	TYR

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Mol	Chain	Res	Type
1	C	685	GLU
1	C	707	SER
1	C	709	LYS
1	C	710	ILE
1	C	725	ARG
1	C	732	LEU
1	C	735	ASN
1	C	742	ARG
1	C	747	VAL
1	C	756	LEU
1	C	771	ILE
1	C	775	LYS
1	C	789	SER
1	C	804	LYS
1	C	806	MET
1	C	808	THR
1	C	811	LEU
1	C	814	GLU
1	C	828	ILE
1	C	835	ARG
1	C	840	ASN
1	C	841	GLN
1	C	842	LYS
1	C	855	ASN
1	C	869	THR
1	C	883	LEU
1	C	908	ASN
1	C	923	ILE
1	C	943	LYS
1	C	944	THR
1	C	945	GLU
1	C	965	LEU
1	C	974	THR
1	C	986	LYS
1	C	988	ASP
1	C	989	SER
1	C	1002	LEU
1	C	1012	LEU
1	C	1038	ARG
1	C	1039	THR
1	C	1042	LEU
1	C	1061	TRP

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Mol	Chain	Res	Type
1	C	1067	SER
1	C	1089	ASN
1	C	1092	THR
1	C	1094	TYR
1	C	1106	LEU
1	C	1108	GLN
1	C	1117	THR
1	C	1120	THR
1	C	1141	LEU
1	C	1150	LYS
1	C	1192	ILE
1	C	1215	ASP
1	C	1226	THR
1	C	1240	GLN
1	C	1243	THR
1	C	1244	SER
1	C	1260	ASP
1	C	1267	LEU
1	C	1270	THR
1	C	1276	ASN
1	C	1282	ASP
1	C	1287	LEU
1	C	1300	ILE
1	C	1309	VAL
1	C	1311	ASN
1	C	1314	LEU
1	C	1318	LEU
1	C	1326	GLN
1	C	1327	GLN
1	C	1336	SER
1	C	1340	GLN
1	C	1342	VAL
1	D	88	PHE
1	D	91	VAL
1	D	100	ILE
1	D	105	LYS
1	D	106	ASN
1	D	119	GLU
1	D	127	ASN
1	D	130	ILE
1	D	142	ASP
1	D	156	ARG

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Mol	Chain	Res	Type
1	D	158	LEU
1	D	178	THR
1	D	184	LYS
1	D	187	VAL
1	D	197	SER
1	D	203	VAL
1	D	204	LEU
1	D	218	ASN
1	D	220	VAL
1	D	223	GLU
1	D	225	LEU
1	D	228	LYS
1	D	231	GLN
1	D	235	ASN
1	D	238	GLN
1	D	239	ARG
1	D	242	LYS
1	D	251	LYS
1	D	257	SER
1	D	259	THR
1	D	272	THR
1	D	300	LEU
1	D	301	LYS
1	D	315	LYS
1	D	319	GLU
1	D	324	LEU
1	D	333	GLU
1	D	342	SER
1	D	350	GLU
1	D	353	THR
1	D	358	VAL
1	D	373	SER
1	D	376	THR
1	D	380	ASN
1	D	384	ILE
1	D	393	LEU
1	D	396	THR
1	D	404	ARG
1	D	405	HIS
1	D	415	LYS
1	D	431	LYS
1	D	436	LYS

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Mol	Chain	Res	Type
1	D	437	LYS
1	D	453	ASN
1	D	458	VAL
1	D	492	THR
1	D	508	LEU
1	D	513	ILE
1	D	523	LEU
1	D	529	ARG
1	D	530	TRP
1	D	562	THR
1	D	567	LYS
1	D	569	ASP
1	D	573	LYS
1	D	609	LEU
1	D	613	MET
1	D	633	ASN
1	D	642	SER
1	D	649	LYS
1	D	662	TYR
1	D	685	GLU
1	D	707	SER
1	D	709	LYS
1	D	710	ILE
1	D	725	ARG
1	D	732	LEU
1	D	735	ASN
1	D	747	VAL
1	D	756	LEU
1	D	771	ILE
1	D	775	LYS
1	D	804	LYS
1	D	807	ILE
1	D	809	GLN
1	D	814	GLU
1	D	816	THR
1	D	817	ARG
1	D	819	VAL
1	D	828	ILE
1	D	835	ARG
1	D	840	ASN
1	D	841	GLN
1	D	842	LYS

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Mol	Chain	Res	Type
1	D	883	LEU
1	D	887	ILE
1	D	908	ASN
1	D	923	ILE
1	D	943	LYS
1	D	944	THR
1	D	945	GLU
1	D	965	LEU
1	D	974	THR
1	D	986	LYS
1	D	989	SER
1	D	993	SER
1	D	1002	LEU
1	D	1012	LEU
1	D	1033	ASP
1	D	1038	ARG
1	D	1039	THR
1	D	1042	LEU
1	D	1067	SER
1	D	1092	THR
1	D	1097	ASN
1	D	1106	LEU
1	D	1108	GLN
1	D	1117	THR
1	D	1120	THR
1	D	1141	LEU
1	D	1150	LYS
1	D	1175	THR
1	D	1192	ILE
1	D	1204	LYS
1	D	1215	ASP
1	D	1220	LYS
1	D	1221	MET
1	D	1226	THR
1	D	1243	THR
1	D	1244	SER
1	D	1260	ASP
1	D	1263	ARG
1	D	1267	LEU
1	D	1270	THR
1	D	1276	ASN
1	D	1282	ASP

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Mol	Chain	Res	Type
1	D	1283	GLN
1	D	1287	LEU
1	D	1300	ILE
1	D	1310	GLU
1	D	1311	ASN
1	D	1314	LEU
1	D	1318	LEU
1	D	1326	GLN
1	D	1327	GLN
1	D	1336	SER
1	D	1340	GLN
1	D	1342	VAL
1	E	57	HIS
1	E	88	PHE
1	E	91	VAL
1	E	98	LEU
1	E	99	ASN
1	E	101	SER
1	E	105	LYS
1	E	106	ASN
1	E	109	ASP
1	E	119	GLU
1	E	125	GLN
1	E	127	ASN
1	E	130	ILE
1	E	142	ASP
1	E	156	ARG
1	E	158	LEU
1	E	178	THR
1	E	184	LYS
1	E	187	VAL
1	E	197	SER
1	E	203	VAL
1	E	204	LEU
1	E	218	ASN
1	E	220	VAL
1	E	222	LYS
1	E	223	GLU
1	E	225	LEU
1	E	228	LYS
1	E	235	ASN
1	E	238	GLN

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Mol	Chain	Res	Type
1	E	239	ARG
1	E	242	LYS
1	E	251	LYS
1	E	257	SER
1	E	259	THR
1	E	268	MET
1	E	272	THR
1	E	300	LEU
1	E	301	LYS
1	E	315	LYS
1	E	319	GLU
1	E	324	LEU
1	E	333	GLU
1	E	334	LYS
1	E	342	SER
1	E	350	GLU
1	E	353	THR
1	E	358	VAL
1	E	373	SER
1	E	376	THR
1	E	380	ASN
1	E	384	ILE
1	E	393	LEU
1	E	396	THR
1	E	404	ARG
1	E	405	HIS
1	E	415	LYS
1	E	431	LYS
1	E	436	LYS
1	E	437	LYS
1	E	453	ASN
1	E	458	VAL
1	E	492	THR
1	E	508	LEU
1	E	513	ILE
1	E	523	LEU
1	E	529	ARG
1	E	530	TRP
1	E	567	LYS
1	E	569	ASP
1	E	573	LYS
1	E	609	LEU

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Mol	Chain	Res	Type
1	E	633	ASN
1	E	642	SER
1	E	649	LYS
1	E	662	TYR
1	E	685	GLU
1	E	707	SER
1	E	709	LYS
1	E	710	ILE
1	E	725	ARG
1	E	732	LEU
1	E	735	ASN
1	E	747	VAL
1	E	756	LEU
1	E	771	ILE
1	E	775	LYS
1	E	790	SER
1	E	804	LYS
1	E	807	ILE
1	E	828	ILE
1	E	835	ARG
1	E	840	ASN
1	E	841	GLN
1	E	842	LYS
1	E	855	ASN
1	E	869	THR
1	E	883	LEU
1	E	908	ASN
1	E	923	ILE
1	E	929	SER
1	E	943	LYS
1	E	944	THR
1	E	945	GLU
1	E	965	LEU
1	E	974	THR
1	E	986	LYS
1	E	989	SER
1	E	993	SER
1	E	1012	LEU
1	E	1033	ASP
1	E	1038	ARG
1	E	1039	THR
1	E	1042	LEU

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Mol	Chain	Res	Type
1	E	1061	TRP
1	E	1067	SER
1	E	1094	TYR
1	E	1095	ASP
1	E	1106	LEU
1	E	1108	GLN
1	E	1117	THR
1	E	1120	THR
1	E	1141	LEU
1	E	1150	LYS
1	E	1188	GLU
1	E	1192	ILE
1	E	1215	ASP
1	E	1220	LYS
1	E	1221	MET
1	E	1226	THR
1	E	1243	THR
1	E	1244	SER
1	E	1260	ASP
1	E	1262	ASN
1	E	1263	ARG
1	E	1267	LEU
1	E	1270	THR
1	E	1276	ASN
1	E	1282	ASP
1	E	1287	LEU
1	E	1300	ILE
1	E	1310	GLU
1	E	1311	ASN
1	E	1318	LEU
1	E	1326	GLN
1	E	1336	SER
1	E	1340	GLN
1	E	1342	VAL
1	E	1346	PHE
1	F	88	PHE
1	F	91	VAL
1	F	94	GLN
1	F	98	LEU
1	F	99	ASN
1	F	101	SER
1	F	106	ASN

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Mol	Chain	Res	Type
1	F	109	ASP
1	F	110	ASP
1	F	119	GLU
1	F	125	GLN
1	F	127	ASN
1	F	130	ILE
1	F	142	ASP
1	F	156	ARG
1	F	158	LEU
1	F	178	THR
1	F	184	LYS
1	F	187	VAL
1	F	197	SER
1	F	203	VAL
1	F	204	LEU
1	F	218	ASN
1	F	220	VAL
1	F	222	LYS
1	F	223	GLU
1	F	225	LEU
1	F	228	LYS
1	F	235	ASN
1	F	238	GLN
1	F	239	ARG
1	F	242	LYS
1	F	251	LYS
1	F	257	SER
1	F	259	THR
1	F	268	MET
1	F	272	THR
1	F	300	LEU
1	F	301	LYS
1	F	315	LYS
1	F	319	GLU
1	F	324	LEU
1	F	333	GLU
1	F	334	LYS
1	F	342	SER
1	F	353	THR
1	F	358	VAL
1	F	373	SER
1	F	376	THR

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Mol	Chain	Res	Type
1	F	380	ASN
1	F	384	ILE
1	F	393	LEU
1	F	396	THR
1	F	404	ARG
1	F	405	HIS
1	F	415	LYS
1	F	431	LYS
1	F	436	LYS
1	F	437	LYS
1	F	453	ASN
1	F	492	THR
1	F	508	LEU
1	F	513	ILE
1	F	523	LEU
1	F	529	ARG
1	F	530	TRP
1	F	567	LYS
1	F	569	ASP
1	F	573	LYS
1	F	609	LEU
1	F	633	ASN
1	F	642	SER
1	F	649	LYS
1	F	662	TYR
1	F	685	GLU
1	F	707	SER
1	F	709	LYS
1	F	710	ILE
1	F	725	ARG
1	F	732	LEU
1	F	735	ASN
1	F	747	VAL
1	F	756	LEU
1	F	771	ILE
1	F	775	LYS
1	F	804	LYS
1	F	807	ILE
1	F	819	VAL
1	F	828	ILE
1	F	835	ARG
1	F	840	ASN

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Mol	Chain	Res	Type
1	F	841	GLN
1	F	842	LYS
1	F	855	ASN
1	F	869	THR
1	F	883	LEU
1	F	908	ASN
1	F	923	ILE
1	F	929	SER
1	F	943	LYS
1	F	944	THR
1	F	945	GLU
1	F	965	LEU
1	F	974	THR
1	F	986	LYS
1	F	989	SER
1	F	993	SER
1	F	1002	LEU
1	F	1012	LEU
1	F	1038	ARG
1	F	1039	THR
1	F	1042	LEU
1	F	1061	TRP
1	F	1067	SER
1	F	1094	TYR
1	F	1095	ASP
1	F	1106	LEU
1	F	1108	GLN
1	F	1117	THR
1	F	1120	THR
1	F	1141	LEU
1	F	1150	LYS
1	F	1188	GLU
1	F	1192	ILE
1	F	1215	ASP
1	F	1220	LYS
1	F	1221	MET
1	F	1226	THR
1	F	1243	THR
1	F	1244	SER
1	F	1246	SER
1	F	1260	ASP
1	F	1263	ARG

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Mol	Chain	Res	Type
1	F	1267	LEU
1	F	1270	THR
1	F	1276	ASN
1	F	1282	ASP
1	F	1283	GLN
1	F	1287	LEU
1	F	1300	ILE
1	F	1301	ARG
1	F	1310	GLU
1	F	1311	ASN
1	F	1314	LEU
1	F	1318	LEU
1	F	1326	GLN
1	F	1336	SER
1	F	1340	GLN
1	F	1342	VAL
1	F	1346	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	94	GLN
1	A	111	ASN
1	A	125	GLN
1	A	126	GLN
1	A	175	ASN
1	A	217	ASN
1	A	235	ASN
1	A	238	GLN
1	A	380	ASN
1	A	391	ASN
1	A	395	GLN
1	A	610	GLN
1	A	629	GLN
1	A	646	ASN
1	A	668	ASN
1	A	681	ASN
1	A	728	GLN
1	A	735	ASN
1	A	737	ASN
1	A	841	GLN

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Mol	Chain	Res	Type
1	A	849	GLN
1	A	854	ASN
1	A	885	ASN
1	A	908	ASN
1	A	909	GLN
1	A	924	ASN
1	A	939	GLN
1	A	947	ASN
1	A	1003	ASN
1	A	1122	ASN
1	A	1327	GLN
1	B	71	ASN
1	B	94	GLN
1	B	97	ASN
1	B	125	GLN
1	B	126	GLN
1	B	175	ASN
1	B	217	ASN
1	B	235	ASN
1	B	238	GLN
1	B	380	ASN
1	B	391	ASN
1	B	610	GLN
1	B	629	GLN
1	B	646	ASN
1	B	681	ASN
1	B	728	GLN
1	B	735	ASN
1	B	737	ASN
1	B	823	ASN
1	B	841	GLN
1	B	849	GLN
1	B	854	ASN
1	B	885	ASN
1	B	908	ASN
1	B	909	GLN
1	B	932	GLN
1	B	939	GLN
1	B	947	ASN
1	B	1122	ASN
1	B	1238	ASN
1	B	1327	GLN

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Mol	Chain	Res	Type
1	C	71	ASN
1	C	94	GLN
1	C	111	ASN
1	C	126	GLN
1	C	235	ASN
1	C	238	GLN
1	C	380	ASN
1	C	391	ASN
1	C	395	GLN
1	C	610	GLN
1	C	646	ASN
1	C	728	GLN
1	C	735	ASN
1	C	737	ASN
1	C	809	GLN
1	C	815	ASN
1	C	841	GLN
1	C	849	GLN
1	C	854	ASN
1	C	908	ASN
1	C	909	GLN
1	C	924	ASN
1	C	939	GLN
1	C	947	ASN
1	C	1327	GLN
1	D	71	ASN
1	D	95	ASN
1	D	111	ASN
1	D	125	GLN
1	D	126	GLN
1	D	175	ASN
1	D	235	ASN
1	D	238	GLN
1	D	380	ASN
1	D	391	ASN
1	D	480	ASN
1	D	610	GLN
1	D	646	ASN
1	D	681	ASN
1	D	728	GLN
1	D	735	ASN
1	D	737	ASN

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Mol	Chain	Res	Type
1	D	810	HIS
1	D	812	ASN
1	D	841	GLN
1	D	849	GLN
1	D	854	ASN
1	D	885	ASN
1	D	908	ASN
1	D	909	GLN
1	D	924	ASN
1	D	939	GLN
1	D	947	ASN
1	D	1097	ASN
1	D	1122	ASN
1	D	1193	GLN
1	D	1327	GLN
1	E	71	ASN
1	E	125	GLN
1	E	126	GLN
1	E	175	ASN
1	E	217	ASN
1	E	235	ASN
1	E	238	GLN
1	E	380	ASN
1	E	391	ASN
1	E	395	GLN
1	E	610	GLN
1	E	646	ASN
1	E	681	ASN
1	E	728	GLN
1	E	733	ASN
1	E	735	ASN
1	E	737	ASN
1	E	841	GLN
1	E	849	GLN
1	E	854	ASN
1	E	885	ASN
1	E	908	ASN
1	E	909	GLN
1	E	939	GLN
1	E	947	ASN
1	E	1122	ASN
1	F	71	ASN

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Mol	Chain	Res	Type
1	F	125	GLN
1	F	126	GLN
1	F	175	ASN
1	F	217	ASN
1	F	235	ASN
1	F	238	GLN
1	F	380	ASN
1	F	391	ASN
1	F	395	GLN
1	F	610	GLN
1	F	646	ASN
1	F	681	ASN
1	F	728	GLN
1	F	733	ASN
1	F	735	ASN
1	F	737	ASN
1	F	841	GLN
1	F	849	GLN
1	F	854	ASN
1	F	885	ASN
1	F	908	ASN
1	F	909	GLN
1	F	939	GLN
1	F	947	ASN
1	F	1122	ASN
1	F	1193	GLN
1	F	1326	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1278/1304 (98%)	0.15	8 (0%) 89 85	13, 49, 106, 165	0
1	B	1275/1304 (97%)	0.28	20 (1%) 72 63	24, 60, 127, 238	0
1	C	1274/1304 (97%)	0.24	21 (1%) 72 63	11, 50, 128, 234	0
1	D	1271/1304 (97%)	0.32	27 (2%) 63 53	18, 58, 132, 228	0
1	E	1262/1304 (96%)	1.91	445 (35%) 0 0	25, 156, 238, 252	0
1	F	1262/1304 (96%)	1.75	431 (34%) 0 0	21, 149, 229, 244	0
All	All	7622/7824 (97%)	0.77	952 (12%) 3 3	11, 68, 224, 252	0

All (952) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	920	PRO	20.2
1	F	836	VAL	14.6
1	F	920	PRO	14.3
1	E	1125	ILE	14.1
1	F	961	TYR	13.9
1	E	626	PRO	13.8
1	F	1125	ILE	13.5
1	E	903	ASN	12.6
1	E	609	LEU	12.5
1	F	659	SER	12.5
1	E	782	SER	12.4
1	F	632	VAL	12.1
1	E	1109	PRO	11.7
1	E	1107	TYR	11.3
1	F	955	GLY	10.9
1	E	957	VAL	10.7
1	E	1119	ASN	10.6
1	E	807	ILE	10.6
1	F	887	ILE	10.5

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Mol	Chain	Res	Type	RSRZ
1	F	921	VAL	10.4
1	E	921	VAL	10.3
1	E	591	ILE	10.2
1	F	922	LEU	10.2
1	E	658	TYR	10.1
1	E	887	ILE	10.1
1	E	1124	LEU	9.9
1	E	257	SER	9.8
1	E	299	PRO	9.7
1	F	884	PRO	9.4
1	F	1106	LEU	9.3
1	E	595	TYR	9.3
1	F	883	LEU	9.3
1	E	1115	TYR	9.2
1	E	625	ASN	9.2
1	F	972	PHE	9.1
1	F	589	LEU	9.1
1	E	256	LEU	8.9
1	E	922	LEU	8.9
1	E	961	TYR	8.8
1	E	599	ASN	8.7
1	E	242	LYS	8.6
1	E	604	PRO	8.6
1	F	956	GLU	8.5
1	E	923	ILE	8.5
1	F	885	ASN	8.5
1	F	1126	GLU	8.5
1	E	1106	LEU	8.3
1	F	886	SER	8.3
1	E	836	VAL	8.2
1	E	799	ILE	8.2
1	E	884	PRO	8.1
1	F	256	LEU	8.1
1	F	877	PRO	8.1
1	F	658	TYR	8.0
1	E	919	ILE	7.9
1	E	1143	LEU	7.9
1	D	1264	LEU	7.9
1	F	803	VAL	7.9
1	E	309	VAL	7.9
1	E	619	PRO	7.8
1	E	1110	ASN	7.8

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Mol	Chain	Res	Type	RSRZ
1	C	1264	LEU	7.8
1	E	968	THR	7.8
1	E	247	LYS	7.8
1	E	392	LEU	7.7
1	F	392	LEU	7.7
1	E	582	GLN	7.7
1	F	899	PHE	7.7
1	E	311	LEU	7.6
1	E	659	SER	7.6
1	A	1264	LEU	7.6
1	F	851	LYS	7.5
1	E	998	VAL	7.5
1	E	566	LEU	7.5
1	E	425	VAL	7.4
1	E	254	GLU	7.4
1	F	853	SER	7.4
1	E	877	PRO	7.3
1	F	310	LYS	7.3
1	F	1127	PRO	7.3
1	F	1000	SER	7.3
1	E	886	SER	7.2
1	E	851	LYS	7.2
1	E	570	GLN	7.2
1	B	1264	LEU	7.1
1	F	878	THR	7.1
1	E	574	HIS	7.1
1	F	626	PRO	7.1
1	F	595	TYR	7.1
1	F	311	LEU	7.0
1	E	1127	PRO	7.0
1	F	575	LEU	6.9
1	E	433	ASP	6.9
1	F	424	LYS	6.9
1	F	1143	LEU	6.8
1	F	603	ILE	6.8
1	D	808	THR	6.8
1	B	809	GLN	6.8
1	E	580	GLN	6.7
1	F	889	PRO	6.7
1	E	668	ASN	6.7
1	F	892	ASP	6.6
1	E	1212	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
1	F	304	ASN	6.6
1	F	590	GLN	6.6
1	E	1112	VAL	6.6
1	F	957	VAL	6.6
1	F	963	ALA	6.5
1	F	818	TRP	6.5
1	F	1124	LEU	6.5
1	F	580	GLN	6.5
1	F	582	GLN	6.5
1	E	806	MET	6.5
1	F	782	SER	6.5
1	E	295	PHE	6.5
1	F	1093	THR	6.4
1	E	1152	LYS	6.4
1	E	859	PHE	6.4
1	F	1119	ASN	6.4
1	F	844	GLY	6.3
1	F	996	THR	6.3
1	F	960	LEU	6.3
1	E	1117	THR	6.3
1	E	571	LEU	6.3
1	E	805	SER	6.2
1	F	625	ASN	6.2
1	F	591	ILE	6.2
1	E	669	TRP	6.2
1	E	893	TRP	6.2
1	F	866	ASN	6.2
1	F	1107	TYR	6.2
1	E	298	LYS	6.2
1	E	883	LEU	6.2
1	F	243	ASP	6.1
1	F	309	VAL	6.1
1	E	424	LYS	6.1
1	F	893	TRP	6.1
1	E	252	GLN	6.1
1	F	923	ILE	6.1
1	E	303	LYS	6.1
1	E	1097	ASN	6.1
1	E	889	PRO	6.1
1	E	253	GLY	6.0
1	E	802	GLY	6.0
1	E	1264	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	803	VAL	6.0
1	F	247	LYS	6.0
1	E	997	LEU	6.0
1	E	593	THR	5.9
1	D	809	GLN	5.9
1	E	1094	TYR	5.9
1	E	885	ASN	5.9
1	E	588	ASP	5.9
1	F	919	ILE	5.9
1	F	824	PHE	5.8
1	F	669	TRP	5.8
1	E	612	GLU	5.8
1	F	558	GLY	5.8
1	E	820	PHE	5.8
1	F	242	LYS	5.8
1	F	624	ASN	5.8
1	F	259	THR	5.7
1	E	300	LEU	5.7
1	F	826	PRO	5.7
1	E	291	LEU	5.7
1	E	1000	SER	5.7
1	F	629	GLN	5.7
1	F	1118	THR	5.7
1	E	1129	ASP	5.7
1	F	974	THR	5.7
1	E	632	VAL	5.7
1	E	761	PHE	5.7
1	E	592	PHE	5.6
1	E	996	THR	5.6
1	F	804	LYS	5.6
1	E	951	LEU	5.6
1	E	434	GLY	5.6
1	F	565	ARG	5.5
1	E	832	ALA	5.5
1	E	589	LEU	5.5
1	E	567	LYS	5.5
1	F	254	GLU	5.5
1	F	398	GLY	5.5
1	E	1108	GLN	5.5
1	E	988	ASP	5.4
1	E	1146	THR	5.4
1	E	987	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	249	SER	5.4
1	E	833	GLY	5.4
1	E	899	PHE	5.3
1	F	593	THR	5.3
1	E	624	ASN	5.3
1	F	278	LYS	5.3
1	E	875	SER	5.3
1	F	832	ALA	5.3
1	F	695	ALA	5.3
1	E	1004	TRP	5.3
1	F	769	PRO	5.3
1	F	387	TYR	5.3
1	F	859	PHE	5.2
1	F	1122	ASN	5.2
1	E	1131	THR	5.2
1	F	792	PRO	5.2
1	A	1093	THR	5.2
1	E	426	GLY	5.2
1	E	1122	ASN	5.2
1	E	1140	LEU	5.2
1	E	853	SER	5.2
1	D	810	HIS	5.2
1	E	393	LEU	5.1
1	B	1259	ILE	5.1
1	E	1116	GLN	5.1
1	E	600	ARG	5.1
1	E	660	GLY	5.1
1	E	575	LEU	5.1
1	F	888	SER	5.1
1	E	243	ASP	5.1
1	F	574	HIS	5.1
1	F	563	VAL	5.1
1	F	587	GLU	5.1
1	F	606	GLY	5.1
1	F	230	THR	5.1
1	E	950	ASN	5.1
1	E	296	ALA	5.1
1	E	615	SER	5.0
1	F	566	LEU	5.0
1	E	830	THR	5.0
1	F	425	VAL	5.0
1	E	906	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	628	ILE	5.0
1	E	771	ILE	5.0
1	E	228	LYS	5.0
1	E	616	LYS	5.0
1	E	1118	THR	5.0
1	F	791	THR	5.0
1	E	947	ASN	5.0
1	E	768	LEU	5.0
1	F	631	ASN	4.9
1	F	652	HIS	4.9
1	E	610	GLN	4.9
1	E	662	TYR	4.9
1	E	652	HIS	4.9
1	E	792	PRO	4.9
1	E	1130	ALA	4.9
1	E	894	ILE	4.9
1	E	1054	ILE	4.9
1	F	295	PHE	4.9
1	F	971	PHE	4.9
1	F	299	PRO	4.9
1	F	229	ALA	4.9
1	E	972	PHE	4.9
1	E	1128	VAL	4.9
1	E	231	GLN	4.9
1	E	1126	GLU	4.8
1	F	607	ALA	4.8
1	E	563	VAL	4.8
1	E	590	GLN	4.8
1	E	801	VAL	4.8
1	E	1093	THR	4.8
1	E	618	GLY	4.8
1	F	246	VAL	4.8
1	F	255	LYS	4.8
1	E	661	LEU	4.8
1	F	599	ASN	4.8
1	E	726	PHE	4.8
1	E	916	LEU	4.8
1	E	584	LEU	4.8
1	F	577	LEU	4.8
1	F	843	ASN	4.8
1	F	302	HIS	4.8
1	F	799	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	394	LEU	4.8
1	E	902	LYS	4.7
1	F	564	PRO	4.7
1	E	888	SER	4.7
1	E	840	ASN	4.7
1	F	835	ARG	4.7
1	F	1002	LEU	4.7
1	E	560	THR	4.7
1	F	998	VAL	4.7
1	C	1283	GLN	4.7
1	E	233	SER	4.7
1	F	248	ASP	4.7
1	F	260	THR	4.7
1	F	692	SER	4.7
1	E	835	ARG	4.7
1	F	628	ILE	4.6
1	E	290	LEU	4.6
1	E	892	ASP	4.6
1	E	963	ALA	4.6
1	E	586	ARG	4.6
1	E	769	PRO	4.6
1	E	428	THR	4.6
1	E	971	PHE	4.6
1	E	804	LYS	4.6
1	F	756	LEU	4.6
1	E	603	ILE	4.6
1	E	234	PHE	4.5
1	E	259	THR	4.5
1	E	955	GLY	4.5
1	F	984	GLY	4.5
1	E	245	PRO	4.5
1	E	956	GLU	4.5
1	E	315	LYS	4.5
1	F	600	ARG	4.5
1	E	688	TYR	4.5
1	F	660	GLY	4.5
1	E	862	ASN	4.5
1	E	796	PHE	4.5
1	F	657	ARG	4.4
1	E	255	LYS	4.4
1	E	908	ASN	4.4
1	E	1121	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	584	LEU	4.4
1	F	965	LEU	4.4
1	E	597	TRP	4.4
1	F	1109	PRO	4.4
1	F	664	TRP	4.4
1	F	404	ARG	4.4
1	E	954	PHE	4.4
1	F	1027	TRP	4.4
1	F	594	PRO	4.3
1	F	231	GLN	4.3
1	E	695	ALA	4.3
1	F	966	LEU	4.3
1	E	965	LEU	4.3
1	F	1144	LEU	4.3
1	F	608	TRP	4.3
1	E	665	GLN	4.3
1	E	904	ASN	4.3
1	A	808	THR	4.3
1	E	640	LEU	4.3
1	E	664	TRP	4.3
1	F	825	SER	4.3
1	E	645	LYS	4.2
1	E	935	LYS	4.2
1	F	388	ASN	4.2
1	F	630	ASP	4.2
1	E	989	SER	4.2
1	E	317	PHE	4.2
1	F	834	TYR	4.2
1	F	1049	LEU	4.2
1	E	232	SER	4.2
1	B	1314	LEU	4.2
1	E	629	GLN	4.2
1	E	828	ILE	4.2
1	F	1204	LYS	4.2
1	E	421	PRO	4.2
1	F	802	GLY	4.2
1	F	962	ASN	4.2
1	F	444	ALA	4.2
1	F	609	LEU	4.2
1	E	959	GLY	4.2
1	F	951	LEU	4.2
1	E	1104	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	397	THR	4.2
1	F	890	THR	4.1
1	E	834	TYR	4.1
1	F	862	ASN	4.1
1	F	924	ASN	4.1
1	F	396	THR	4.1
1	F	298	LYS	4.1
1	F	585	LEU	4.1
1	F	586	ARG	4.1
1	F	903	ASN	4.1
1	F	620	HIS	4.1
1	E	793	LEU	4.1
1	F	559	ASP	4.1
1	F	552	ALA	4.0
1	F	726	PHE	4.0
1	E	898	THR	4.0
1	E	389	ALA	4.0
1	F	908	ASN	4.0
1	E	297	LYS	4.0
1	F	897	LEU	4.0
1	F	1182	ILE	4.0
1	F	553	GLY	4.0
1	E	229	ALA	4.0
1	E	878	THR	4.0
1	E	585	LEU	4.0
1	E	895	ASN	4.0
1	F	1108	GLN	4.0
1	E	897	LEU	4.0
1	E	667	PHE	4.0
1	E	1182	ILE	4.0
1	F	245	PRO	3.9
1	F	303	LYS	3.9
1	E	641	ILE	3.9
1	F	588	ASP	3.9
1	F	654	TYR	3.9
1	E	608	TRP	3.9
1	F	988	ASP	3.9
1	E	429	ASP	3.9
1	E	842	LYS	3.9
1	F	619	PRO	3.9
1	E	583	GLY	3.9
1	F	994	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	1309	VAL	3.9
1	E	577	LEU	3.9
1	E	302	HIS	3.9
1	F	1205	GLN	3.9
1	D	1345	PRO	3.8
1	F	592	PHE	3.8
1	E	246	VAL	3.8
1	E	294	ASP	3.8
1	E	901	ASN	3.8
1	F	393	LEU	3.8
1	E	1207	ASN	3.8
1	F	1110	ASN	3.8
1	F	597	TRP	3.8
1	F	394	LEU	3.8
1	E	764	PHE	3.8
1	F	941	TRP	3.8
1	F	926	SER	3.8
1	F	768	LEU	3.8
1	E	781	PRO	3.8
1	F	225	LEU	3.8
1	E	868	VAL	3.8
1	F	667	PHE	3.8
1	E	282	GLU	3.8
1	F	1042	LEU	3.8
1	E	876	LYS	3.7
1	E	994	SER	3.7
1	F	906	GLN	3.7
1	F	554	THR	3.7
1	F	987	ALA	3.7
1	E	670	SER	3.7
1	F	1141	LEU	3.7
1	E	278	LYS	3.7
1	F	1115	TYR	3.7
1	F	857	THR	3.7
1	F	421	PRO	3.7
1	E	313	ALA	3.7
1	F	845	ILE	3.7
1	F	801	VAL	3.7
1	F	848	GLU	3.7
1	E	237	THR	3.6
1	F	989	SER	3.6
1	F	427	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	225	LEU	3.6
1	F	604	PRO	3.6
1	E	536	ARG	3.6
1	F	691	ASN	3.6
1	F	776	PRO	3.6
1	F	1056	TRP	3.6
1	E	1123	LYS	3.6
1	B	810	HIS	3.6
1	F	656	TYR	3.6
1	E	551	LEU	3.6
1	E	1141	LEU	3.6
1	F	997	LEU	3.6
1	F	855	ASN	3.6
1	E	843	ASN	3.6
1	F	551	LEU	3.6
1	B	808	THR	3.6
1	E	753	GLY	3.6
1	F	1121	TYR	3.6
1	E	960	LEU	3.5
1	E	436	LYS	3.5
1	F	764	PHE	3.5
1	F	964	ALA	3.5
1	F	1097	ASN	3.5
1	E	553	GLY	3.5
1	E	275	LYS	3.5
1	E	605	VAL	3.5
1	F	1207	ASN	3.5
1	F	317	PHE	3.5
1	E	683	VAL	3.5
1	F	262	SER	3.5
1	D	1240	GLN	3.5
1	E	565	ARG	3.5
1	D	1259	ILE	3.5
1	E	692	SER	3.5
1	F	771	ILE	3.5
1	F	898	THR	3.5
1	F	882	ALA	3.5
1	E	279	VAL	3.5
1	F	234	PHE	3.5
1	E	1002	LEU	3.5
1	F	222	LYS	3.5
1	F	1105	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	383	GLY	3.5
1	E	958	ASN	3.5
1	E	1153	LEU	3.5
1	F	641	ILE	3.5
1	F	672	LYS	3.5
1	E	431	LYS	3.4
1	E	1213	ILE	3.4
1	E	844	GLY	3.4
1	F	279	VAL	3.4
1	E	587	GLU	3.4
1	E	653	VAL	3.4
1	E	666	LEU	3.4
1	E	880	TYR	3.4
1	E	770	TRP	3.4
1	F	1188	GLU	3.4
1	D	1314	LEU	3.4
1	F	571	LEU	3.4
1	E	236	PRO	3.4
1	E	1027	TRP	3.4
1	E	819	VAL	3.4
1	F	949	GLY	3.4
1	F	403	ARG	3.4
1	F	567	LYS	3.4
1	F	227	VAL	3.4
1	F	538	ALA	3.4
1	F	390	ARG	3.4
1	F	876	LYS	3.4
1	F	1153	LEU	3.4
1	E	240	LEU	3.4
1	F	655	PRO	3.4
1	F	273	ARG	3.4
1	F	226	GLU	3.3
1	E	693	LEU	3.3
1	E	552	ALA	3.3
1	E	396	THR	3.3
1	F	696	ALA	3.3
1	E	1134	ALA	3.3
1	F	894	ILE	3.3
1	E	1263	ARG	3.3
1	F	775	LYS	3.3
1	E	573	LYS	3.3
1	F	308	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	1015	ILE	3.3
1	F	952	PRO	3.3
1	F	1046	LEU	3.3
1	E	630	ASP	3.3
1	F	627	ASP	3.3
1	D	826	PRO	3.3
1	F	723	ALA	3.3
1	F	688	TYR	3.3
1	F	976	THR	3.3
1	F	767	PHE	3.3
1	F	1140	LEU	3.3
1	F	937	SER	3.3
1	E	241	GLN	3.3
1	F	1240	GLN	3.3
1	F	986	LYS	3.3
1	E	627	ASP	3.3
1	E	281	VAL	3.3
1	E	861	PRO	3.3
1	F	622	PHE	3.3
1	F	232	SER	3.3
1	F	830	THR	3.3
1	B	815	ASN	3.2
1	F	481	PRO	3.2
1	E	969	TYR	3.2
1	E	728	GLN	3.2
1	E	852	PRO	3.2
1	F	618	GLY	3.2
1	E	1099	THR	3.2
1	E	274	ALA	3.2
1	F	746	VAL	3.2
1	F	1191	SER	3.2
1	D	1289	VAL	3.2
1	F	995	SER	3.2
1	F	274	ALA	3.2
1	F	1104	PHE	3.2
1	F	221	VAL	3.2
1	F	1004	TRP	3.2
1	E	100	ILE	3.2
1	F	925	LYS	3.2
1	E	277	LEU	3.2
1	F	954	PHE	3.2
1	F	990	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	1288	LEU	3.2
1	F	1043	GLY	3.2
1	F	1142	LYS	3.2
1	E	952	PRO	3.1
1	E	983	ILE	3.1
1	F	915	LEU	3.1
1	F	401	ASN	3.1
1	F	916	LEU	3.1
1	E	432	LYS	3.1
1	F	261	ALA	3.1
1	F	301	LYS	3.1
1	F	661	LEU	3.1
1	E	648	ASP	3.1
1	E	382	HIS	3.1
1	E	826	PRO	3.1
1	F	1137	MET	3.1
1	E	777	PHE	3.1
1	E	550	VAL	3.1
1	E	1144	LEU	3.1
1	E	578	VAL	3.1
1	E	284	GLY	3.1
1	C	1263	ARG	3.1
1	F	690	PRO	3.1
1	E	391	ASN	3.1
1	F	670	SER	3.1
1	E	1029	ILE	3.1
1	F	975	ASN	3.1
1	F	428	THR	3.1
1	E	621	TYR	3.0
1	F	447	PHE	3.0
1	E	330	ILE	3.0
1	F	940	LYS	3.0
1	E	694	PHE	3.0
1	F	852	PRO	3.0
1	E	280	GLU	3.0
1	E	397	THR	3.0
1	E	126	GLN	3.0
1	E	642	SER	3.0
1	E	974	THR	3.0
1	F	983	ILE	3.0
1	F	503	TRP	3.0
1	F	1031	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	949	GLY	3.0
1	F	275	LYS	3.0
1	E	564	PRO	3.0
1	E	620	HIS	3.0
1	F	781	PRO	3.0
1	F	433	ASP	3.0
1	F	753	GLY	3.0
1	E	1111	LYS	3.0
1	E	235	ASN	3.0
1	E	918	THR	3.0
1	B	268	MET	3.0
1	F	754	PRO	3.0
1	E	598	ALA	3.0
1	F	653	VAL	3.0
1	F	323	PRO	3.0
1	E	510	GLY	3.0
1	C	807	ILE	3.0
1	E	227	VAL	3.0
1	E	864	ASP	3.0
1	F	644	TYR	3.0
1	F	569	ASP	2.9
1	E	390	ARG	2.9
1	E	907	ARG	2.9
1	E	508	LEU	2.9
1	F	761	PHE	2.9
1	E	307	GLY	2.9
1	E	1046	LEU	2.9
1	E	995	SER	2.9
1	E	845	ILE	2.9
1	F	1117	THR	2.9
1	F	568	TYR	2.9
1	F	1083	ALA	2.9
1	F	1146	THR	2.9
1	E	596	GLY	2.9
1	C	1259	ILE	2.9
1	E	855	ASN	2.9
1	E	1262	ASN	2.9
1	E	1100	LEU	2.9
1	E	579	ALA	2.9
1	E	719	ALA	2.9
1	F	252	GLN	2.9
1	D	1262	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	985	PHE	2.9
1	E	310	LYS	2.9
1	F	693	LEU	2.9
1	F	109	ASP	2.9
1	C	810	HIS	2.9
1	F	1044	ILE	2.8
1	F	395	GLN	2.8
1	D	1344	GLN	2.8
1	E	910	LEU	2.8
1	D	1263	ARG	2.8
1	E	484	ILE	2.8
1	E	482	LEU	2.8
1	E	569	ASP	2.8
1	F	985	PHE	2.8
1	F	958	ASN	2.8
1	F	281	VAL	2.8
1	F	850	VAL	2.8
1	E	780	SER	2.8
1	E	1210	GLU	2.8
1	D	1285	VAL	2.8
1	F	249	SER	2.8
1	E	558	GLY	2.8
1	E	860	ASP	2.8
1	F	1009	VAL	2.8
1	E	941	TRP	2.7
1	F	321	TRP	2.7
1	B	805	SER	2.7
1	F	861	PRO	2.7
1	F	294	ASP	2.7
1	E	993	SER	2.7
1	E	401	ASN	2.7
1	E	890	THR	2.7
1	F	228	LYS	2.7
1	F	315	LYS	2.7
1	E	400	PHE	2.7
1	B	106	ASN	2.7
1	F	429	ASP	2.7
1	E	696	ALA	2.7
1	E	403	ARG	2.7
1	A	809	GLN	2.7
1	F	1094	TYR	2.7
1	E	430	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	793	LEU	2.7
1	F	426	GLY	2.7
1	E	387	TYR	2.7
1	E	848	GLU	2.7
1	F	910	LEU	2.7
1	E	301	LYS	2.7
1	E	999	GLY	2.7
1	D	106	ASN	2.7
1	E	623	LEU	2.7
1	F	290	LEU	2.6
1	F	780	SER	2.6
1	F	860	ASP	2.6
1	E	617	PHE	2.6
1	E	449	ALA	2.6
1	F	233	SER	2.6
1	E	924	ASN	2.6
1	A	816	THR	2.6
1	B	259	THR	2.6
1	F	1187	LYS	2.6
1	B	230	THR	2.6
1	E	408	TRP	2.6
1	E	823	ASN	2.6
1	F	100	ILE	2.6
1	F	443	ILE	2.6
1	D	1265	PHE	2.6
1	E	1066	GLY	2.6
1	E	1024	LEU	2.6
1	E	1211	ILE	2.6
1	F	1152	LYS	2.6
1	E	690	PRO	2.6
1	E	395	GLN	2.6
1	F	909	GLN	2.6
1	E	230	THR	2.6
1	F	1003	ASN	2.6
1	F	283	ARG	2.6
1	E	639	ALA	2.6
1	F	933	PHE	2.6
1	B	806	MET	2.6
1	F	615	SER	2.6
1	F	880	TYR	2.5
1	F	856	SER	2.5
1	F	1189	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	986	LYS	2.5
1	E	905	PRO	2.5
1	E	568	TYR	2.5
1	E	607	ALA	2.5
1	F	576	ASN	2.5
1	F	318	THR	2.5
1	E	283	ARG	2.5
1	F	1213	ILE	2.5
1	C	1262	ASN	2.5
1	E	416	ALA	2.5
1	E	276	ALA	2.5
1	F	639	ALA	2.5
1	F	1155	LYS	2.5
1	B	1262	ASN	2.5
1	F	668	ASN	2.5
1	E	944	THR	2.5
1	F	579	ALA	2.5
1	F	689	ALA	2.5
1	E	729	LEU	2.5
1	F	968	THR	2.5
1	E	654	TYR	2.5
1	F	550	VAL	2.5
1	F	1112	VAL	2.5
1	F	796	PHE	2.5
1	E	962	ASN	2.5
1	E	644	TYR	2.5
1	E	756	LEU	2.5
1	D	1270	THR	2.5
1	F	633	ASN	2.5
1	F	907	ARG	2.5
1	C	1272	LEU	2.5
1	E	520	LEU	2.5
1	F	1116	GLN	2.5
1	E	1078	LEU	2.5
1	F	833	GLY	2.5
1	F	473	ALA	2.5
1	F	1264	LEU	2.5
1	D	1268	PRO	2.5
1	F	257	SER	2.5
1	F	875	SER	2.5
1	E	1065	LYS	2.4
1	C	97	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	882	ALA	2.4
1	E	562	THR	2.4
1	E	931	ASP	2.4
1	E	912	LEU	2.4
1	F	797	SER	2.4
1	F	912	LEU	2.4
1	F	276	ALA	2.4
1	F	694	PHE	2.4
1	E	308	GLU	2.4
1	E	1190	THR	2.4
1	E	1092	THR	2.4
1	F	939	GLN	2.4
1	E	673	LEU	2.4
1	E	1001	GLY	2.4
1	E	262	SER	2.4
1	F	250	SER	2.4
1	E	866	ASN	2.4
1	F	904	ASN	2.4
1	F	1050	GLN	2.4
1	E	911	LEU	2.4
1	F	917	GLY	2.4
1	A	993	SER	2.4
1	F	570	GLN	2.4
1	D	805	SER	2.4
1	F	642	SER	2.4
1	F	382	HIS	2.4
1	F	241	GLN	2.4
1	F	849	GLN	2.4
1	F	646	ASN	2.4
1	C	1297	GLN	2.4
1	E	576	ASN	2.4
1	F	1098	PRO	2.4
1	E	1113	LYS	2.4
1	F	616	LYS	2.4
1	E	791	THR	2.4
1	E	1049	LEU	2.4
1	F	291	LEU	2.4
1	F	795	THR	2.4
1	E	1010	GLY	2.3
1	E	990	SER	2.3
1	F	805	SER	2.3
1	C	1284	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	473	ALA	2.3
1	F	662	TYR	2.3
1	E	765	LEU	2.3
1	F	944	THR	2.3
1	E	1031	PHE	2.3
1	E	1102	PRO	2.3
1	C	1269	VAL	2.3
1	E	606	GLY	2.3
1	F	864	ASP	2.3
1	F	623	LEU	2.3
1	F	959	GLY	2.3
1	F	1128	VAL	2.3
1	F	617	PHE	2.3
1	C	1096	THR	2.3
1	E	385	TRP	2.3
1	E	404	ARG	2.3
1	F	307	GLY	2.3
1	E	709	LYS	2.3
1	F	772	GLY	2.3
1	F	999	GLY	2.3
1	E	258	GLU	2.3
1	E	312	GLU	2.3
1	F	770	TRP	2.3
1	F	1206	ASN	2.3
1	E	503	TRP	2.3
1	E	1225	LEU	2.3
1	F	914	SER	2.3
1	F	829	TRP	2.3
1	F	643	SER	2.3
1	E	314	GLU	2.2
1	B	851	LYS	2.2
1	D	259	THR	2.2
1	E	824	PHE	2.2
1	E	1081	PRO	2.2
1	F	601	PRO	2.2
1	D	955	GLY	2.2
1	C	1314	LEU	2.2
1	C	1093	THR	2.2
1	E	928	ASP	2.2
1	F	1262	ASN	2.2
1	F	536	ARG	2.2
1	F	932	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	867	LYS	2.2
1	E	966	LEU	2.2
1	F	445	LEU	2.2
1	E	559	ASP	2.2
1	F	297	LYS	2.2
1	F	583	GLY	2.2
1	F	1001	GLY	2.2
1	D	806	MET	2.2
1	F	1091	SER	2.2
1	F	435	PHE	2.2
1	F	312	GLU	2.2
1	E	444	ALA	2.2
1	F	506	ALA	2.2
1	E	216	LEU	2.2
1	F	277	LEU	2.2
1	E	713	GLY	2.2
1	F	236	PRO	2.2
1	F	1006	SER	2.2
1	C	1115	TYR	2.2
1	E	846	PRO	2.2
1	F	665	GLN	2.2
1	E	976	THR	2.2
1	F	296	ALA	2.2
1	E	1058	ASP	2.2
1	E	1020	PHE	2.2
1	F	973	GLY	2.2
1	D	1334	ALA	2.2
1	E	841	GLN	2.2
1	B	1097	ASN	2.2
1	F	470	ASN	2.2
1	B	1263	ARG	2.2
1	F	817	ARG	2.2
1	F	389	ALA	2.2
1	C	1091	SER	2.1
1	D	1324	GLN	2.1
1	E	874	SER	2.1
1	A	996	THR	2.1
1	F	1045	THR	2.1
1	E	847	PHE	2.1
1	E	441	SER	2.1
1	C	1346	PHE	2.1
1	E	532	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	211	LEU	2.1
1	F	1224	LYS	2.1
1	E	926	SER	2.1
1	A	1263	ARG	2.1
1	F	1130	ALA	2.1
1	E	1096	THR	2.1
1	E	1181	ASN	2.1
1	F	710	ILE	2.1
1	E	1042	LEU	2.1
1	E	1208	LYS	2.1
1	E	680	ALA	2.1
1	C	840	ASN	2.1
1	E	454	ILE	2.1
1	E	1032	THR	2.1
1	F	217	ASN	2.1
1	F	831	GLY	2.1
1	F	621	TYR	2.1
1	E	248	ASP	2.1
1	F	578	VAL	2.1
1	B	812	ASN	2.1
1	C	815	ASN	2.1
1	F	755	ASN	2.1
1	E	827	ASP	2.1
1	E	1095	ASP	2.1
1	D	1312	GLN	2.1
1	F	1211	ILE	2.1
1	F	1100	LEU	2.1
1	E	720	GLU	2.1
1	E	773	ASN	2.0
1	E	711	PHE	2.0
1	B	1093	THR	2.0
1	E	684	ASN	2.0
1	F	946	THR	2.0
1	F	1078	LEU	2.0
1	F	1225	LEU	2.0
1	E	891	SER	2.0
1	F	931	ASP	2.0
1	F	240	LEU	2.0
1	E	671	ASN	2.0
1	F	777	PHE	2.0
1	E	1090	SER	2.0
1	F	467	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	304	ASN	2.0
1	F	950	ASN	2.0
1	E	1105	GLN	2.0
1	B	1272	LEU	2.0
1	E	1091	SER	2.0
1	F	505	TYR	2.0
1	F	1068	TYR	2.0
1	C	1089	ASN	2.0
1	F	1007	GLN	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.