Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 10:27 AM EST

PDB ID	:	3PIE
Title	:	Crystal structure of the 5'->3' exoribonuclease Xrn1, E178Q mutant
Authors	:	Chang, J.H.; Xiang, S.; Tong, L.
Deposited on	:	2010-11-06
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

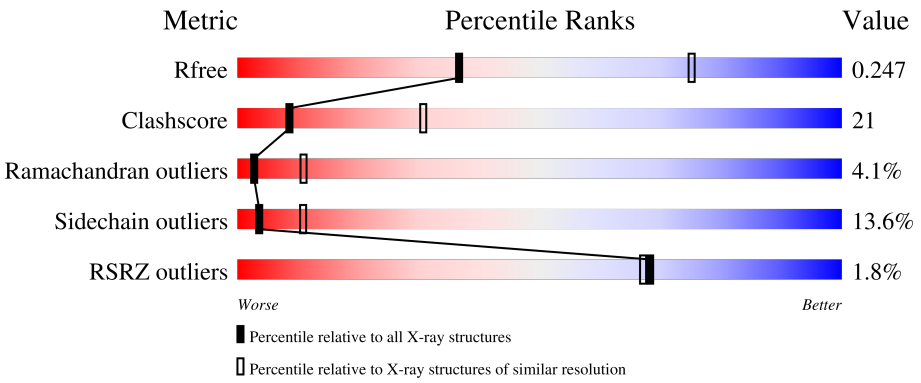
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1155	.% 54% 31% 6% • 8%
1	B	1155	2% 53% 32% 6% • 9%
1	C	1155	2% 56% 29% 7% 8%
1	D	1155	2% 50% 31% 7% • 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 34009 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 5'->3' EXORIBONUCLEASE (Xrn1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1057	8549	5509	1438	1579	23	0	0	0
1	B	1056	8535	5501	1436	1575	23	0	0	0
1	C	1066	8605	5543	1446	1593	23	0	0	0
1	D	1023	8320	5365	1397	1535	23	0	0	0

There are 188 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	GLN	GLU	engineered mutation	UNP Q6CJ09
A	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	473	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	478	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	483	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1246	LEU	-	expression tag	UNP Q6CJ09
A	1247	GLU	-	expression tag	UNP Q6CJ09
A	1248	HIS	-	expression tag	UNP Q6CJ09
A	1249	HIS	-	expression tag	UNP Q6CJ09
A	1250	HIS	-	expression tag	UNP Q6CJ09
A	1251	HIS	-	expression tag	UNP Q6CJ09
A	1252	HIS	-	expression tag	UNP Q6CJ09
A	1253	HIS	-	expression tag	UNP Q6CJ09
B	178	GLN	GLU	engineered mutation	UNP Q6CJ09
B	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	473	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	478	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	483	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1246	LEU	-	expression tag	UNP Q6CJ09
B	1247	GLU	-	expression tag	UNP Q6CJ09
B	1248	HIS	-	expression tag	UNP Q6CJ09
B	1249	HIS	-	expression tag	UNP Q6CJ09
B	1250	HIS	-	expression tag	UNP Q6CJ09
B	1251	HIS	-	expression tag	UNP Q6CJ09
B	1252	HIS	-	expression tag	UNP Q6CJ09
B	1253	HIS	-	expression tag	UNP Q6CJ09
C	178	GLN	GLU	engineered mutation	UNP Q6CJ09
C	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	473	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	478	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
C	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	483	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1246	LEU	-	expression tag	UNP Q6CJ09
C	1247	GLU	-	expression tag	UNP Q6CJ09
C	1248	HIS	-	expression tag	UNP Q6CJ09
C	1249	HIS	-	expression tag	UNP Q6CJ09
C	1250	HIS	-	expression tag	UNP Q6CJ09
C	1251	HIS	-	expression tag	UNP Q6CJ09
C	1252	HIS	-	expression tag	UNP Q6CJ09
C	1253	HIS	-	expression tag	UNP Q6CJ09
D	178	GLN	GLU	engineered mutation	UNP Q6CJ09
D	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	473	UNK	-	SEE REMARK 999	UNP Q6CJ09

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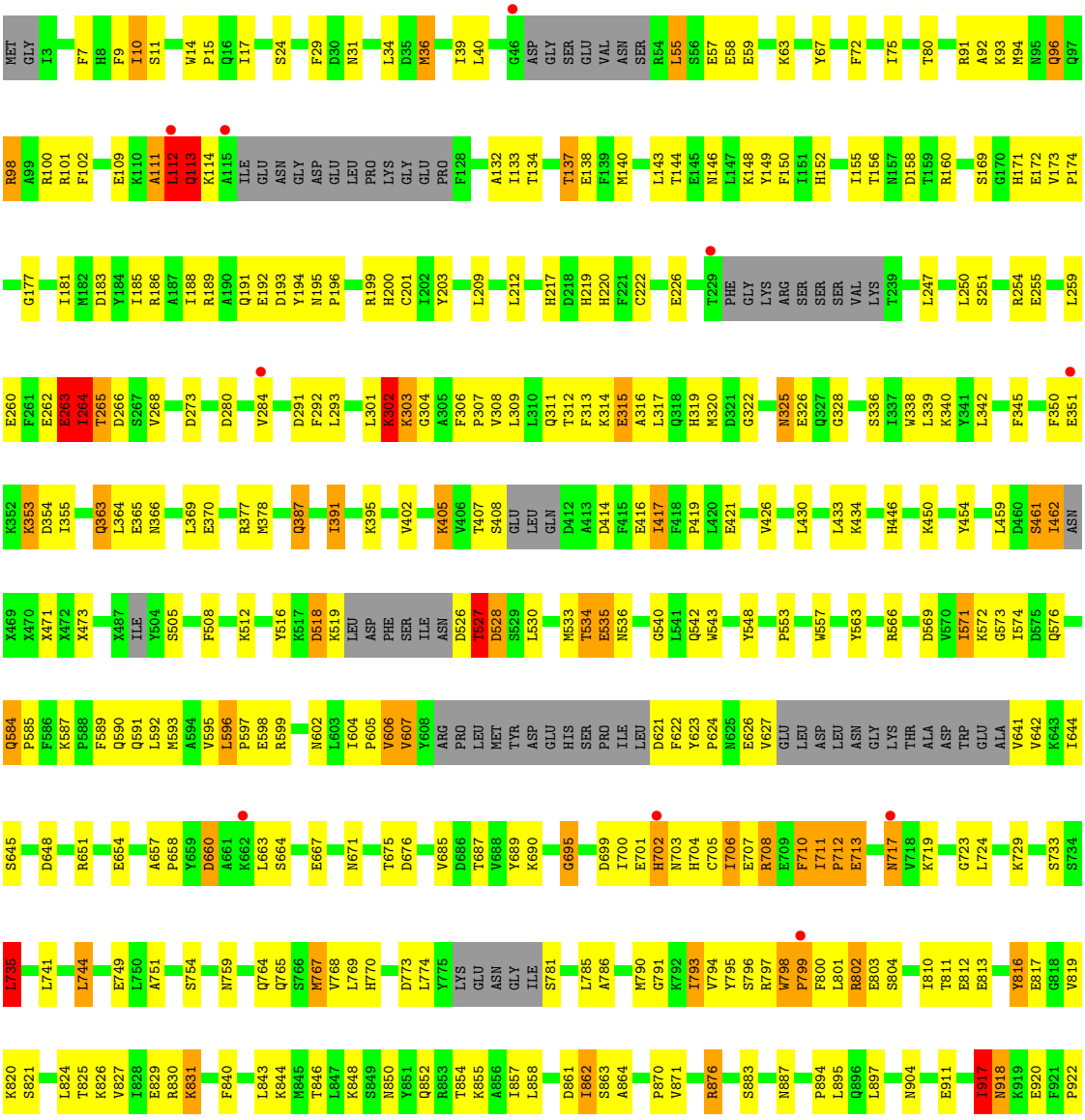
Chain	Residue	Modelled	Actual	Comment	Reference
D	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	478	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	483	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1246	LEU	-	expression tag	UNP Q6CJ09
D	1247	GLU	-	expression tag	UNP Q6CJ09
D	1248	HIS	-	expression tag	UNP Q6CJ09
D	1249	HIS	-	expression tag	UNP Q6CJ09
D	1250	HIS	-	expression tag	UNP Q6CJ09
D	1251	HIS	-	expression tag	UNP Q6CJ09
D	1252	HIS	-	expression tag	UNP Q6CJ09
D	1253	HIS	-	expression tag	UNP Q6CJ09

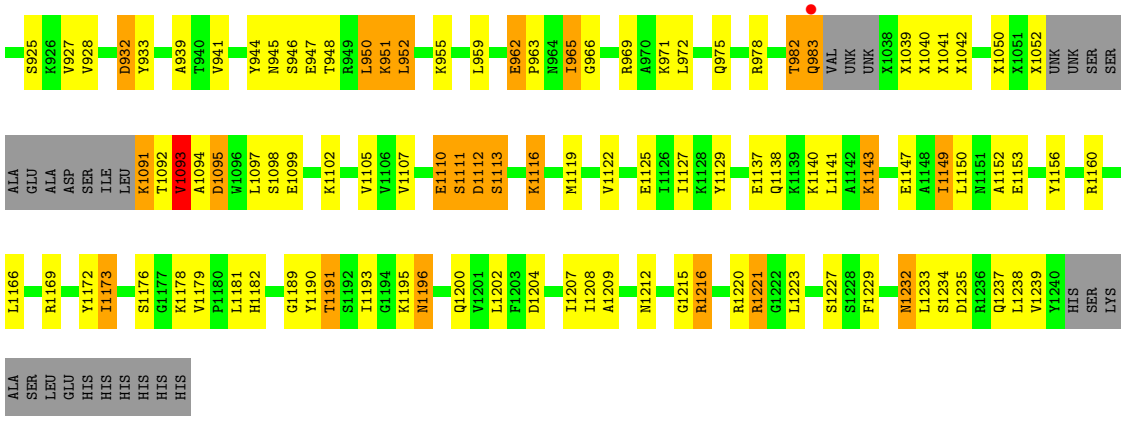
3 Residue-property plots (i)

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

- Molecule 1: 5'->3' EXORIBONUCLEASE (Xrn1)

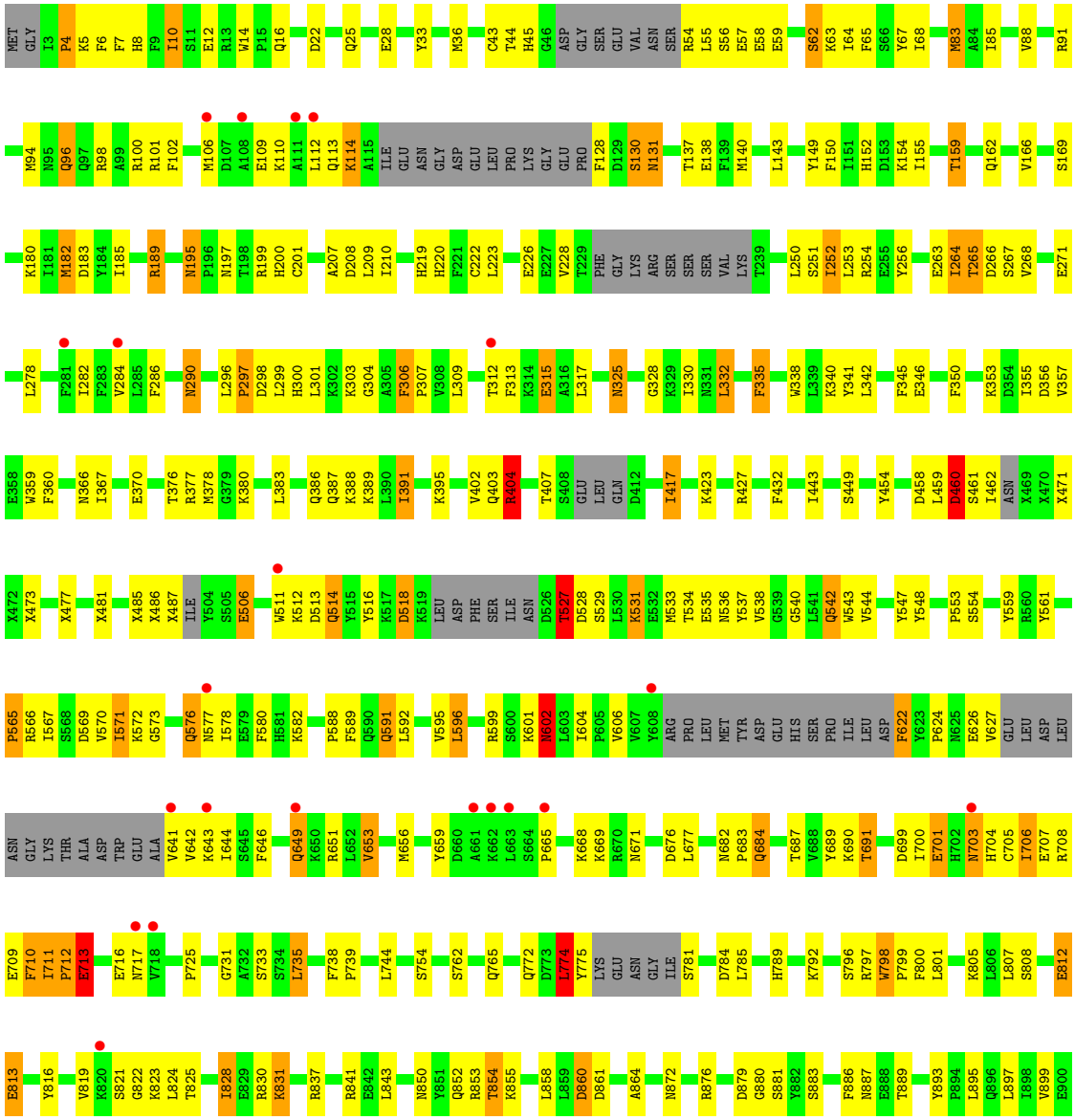
Chain A:

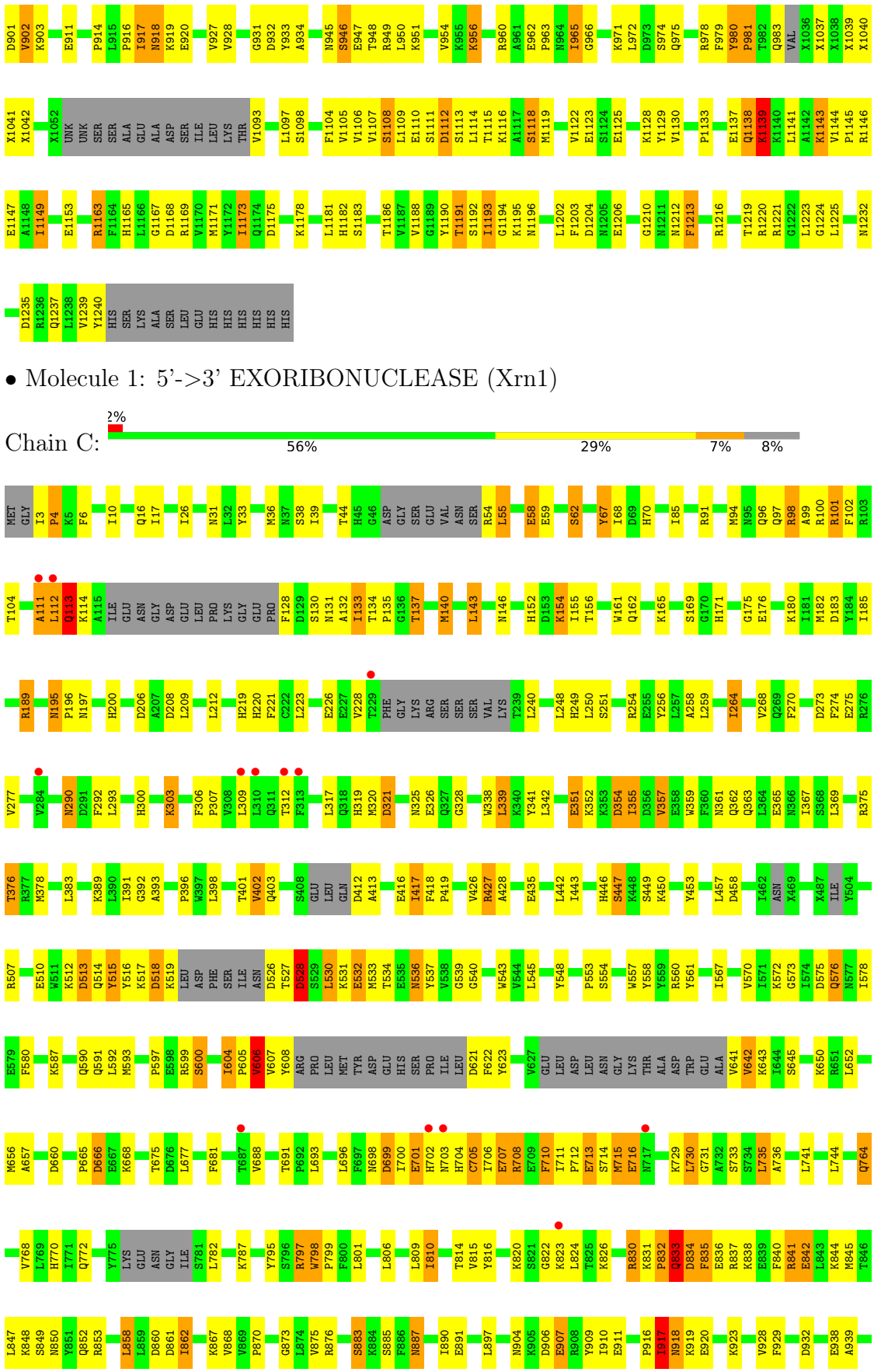




• Molecule 1: 5'->3' EXORIBONUCLEASE (Xrn1)

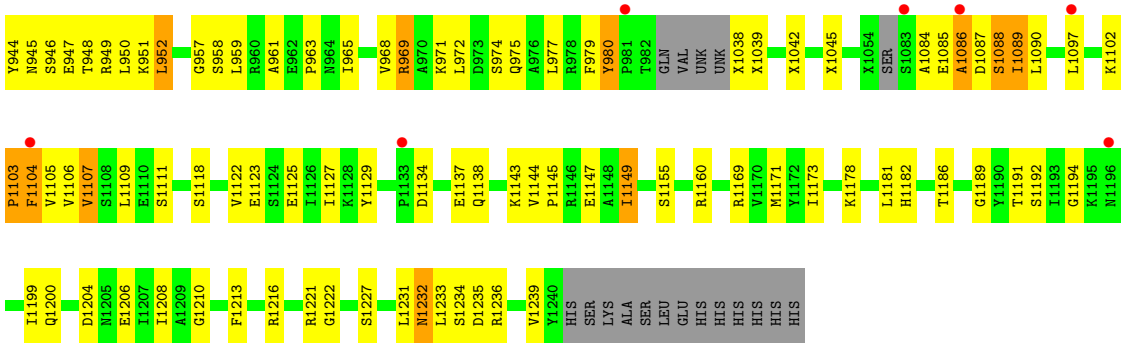
Chain B:





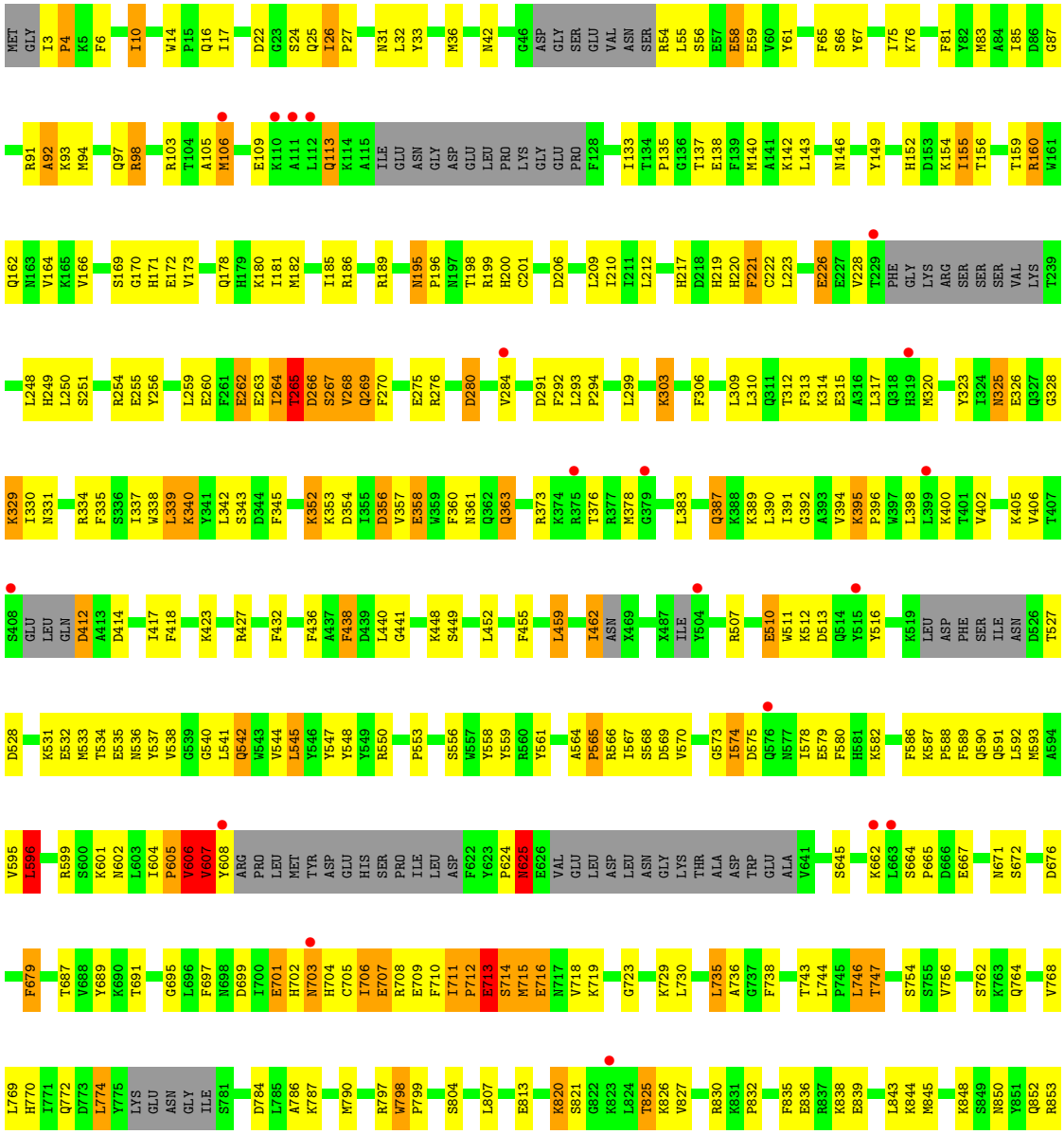
• Molecule 1: 5'->3' EXORIBONUCLEASE (Xrn1)

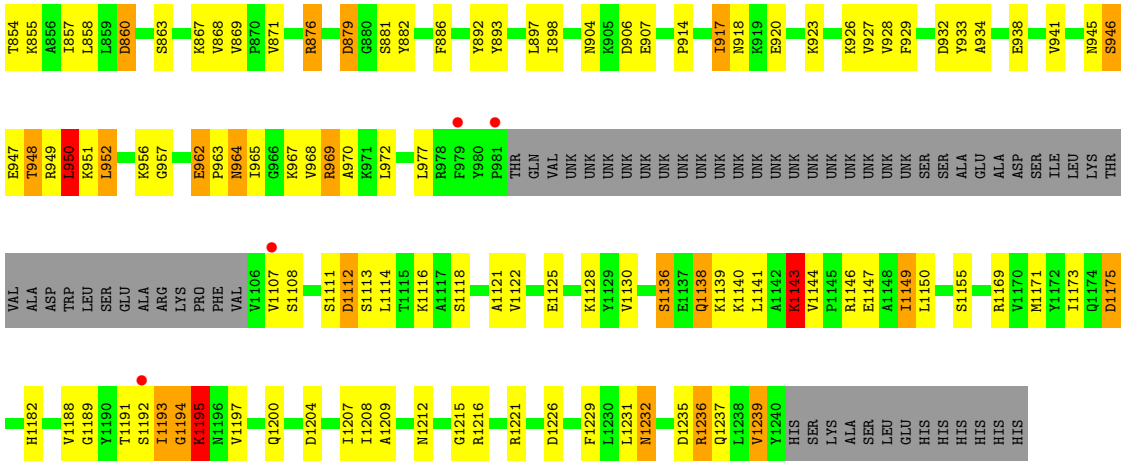
Chain C: 2% 56% 29% 7% 8%



- Molecule 1: 5'->3' EXORIBONUCLEASE (Xrn1)

Chain D:




T854 K855 A856 I857 L858 L859 D860 S863 K867 V868 V869 P870 V871 R876 D879 G880 S881 Y882 F886 Y892 Y893 L897 I898 N904 K905 D906 E907 P914 I917 N918 K919 E920 K923 K926 V927 V928 F929 D932 Y933 A934 E938 V941 N945 S946
E947 T948 R949 L950 K951 L952 K956 G957 E962 P963 N964 I965 G966 K967 V968 R969 A970 K971 L972 L977 R978 F979 Y980 P981 THR GLN VAL UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK SER SER ALA GLU ALA ASP SER ILE LEU LYS THR
VAL ALA ASP TRP LEU SER GLU ALA ARG LYS PRO PHE VAL V1106 V1107 S1108 S1111 D1112 S1113 L1114 T1115 K1116 A1117 S1118 A1121 V1122 E1125 K1128 Y1129 V1130 S1136 E1137 Q1138 K1139 K1140 L1141 A1142 K1143 V1144 P1145 R1146 E1147 A1148 I1149 L1150 S1155 R1169 V1170 M1171 Y1172 I1173 Q1174 D1175
H1182 V1188 G1189 Y1190 T1191 S1192 I1193 G1194 K1195 N1196 V1197 Q1200 D1204 I1207 I1208 A1209 N1212 G1215 R1216 R1221 D1226 F1229 L1230 L1231 N1232 D1235 R1236 Q1237 L1238 V1239 Y1240 HIS SER LYS ALA SER LEU GLU HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	115.72Å 132.29Å 143.89Å 110.07° 105.70° 103.75°	Depositor
Resolution (Å)	30.00 – 2.90 29.49 – 2.88	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-2.90) 96.4 (29.49-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.49 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.241 , 0.305 0.244 , 0.247	Depositor DCC
R_{free} test set	7868 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	34009	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.81	3/8567 (0.0%)	0.83	4/11553 (0.0%)
1	B	0.81	2/8543 (0.0%)	0.83	2/11521 (0.0%)
1	C	0.74	3/8613 (0.0%)	0.79	4/11616 (0.0%)
1	D	0.66	0/8409	0.76	3/11337 (0.0%)
All	All	0.76	8/34132 (0.0%)	0.80	13/46027 (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	C	0	2
1	D	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	705	CYS	CB-SG	8.69	1.97	1.82
1	C	1086	ALA	C-O	6.39	1.35	1.23
1	B	709	GLU	CB-CG	6.38	1.64	1.52
1	A	598	GLU	CB-CG	5.65	1.62	1.52
1	C	1089	ILE	C-O	5.48	1.33	1.23
1	A	598	GLU	CG-CD	5.38	1.60	1.51
1	C	705	CYS	CB-SG	5.32	1.91	1.82
1	B	813	GLU	CG-CD	5.13	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	240	LEU	CA-CB-CG	6.40	130.02	115.30
1	D	774	LEU	CA-CB-CG	6.27	129.72	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	264	ILE	CB-CA-C	-6.16	99.28	111.60
1	B	860	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	950	LEU	CA-CB-CG	5.52	128.00	115.30
1	C	710	PHE	N-CA-CB	-5.43	100.83	110.60
1	D	923	LYS	CD-CE-NZ	5.38	124.06	111.70
1	B	1173	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	D	950	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	774	LEU	CA-CB-CG	5.17	127.19	115.30
1	C	906	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	10	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	A	264	ILE	CB-CA-C	-5.06	101.49	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	797	ARG	Peptide
1	C	980	TYR	Peptide
1	D	860	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8549	0	8404	377	0
1	B	8535	0	8385	351	0
1	C	8605	0	8450	346	0
1	D	8320	0	8233	327	0
All	All	34009	0	33472	1394	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 21.

All (1394) 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:A:744:LEU:HD22	1:A:798:TRP:CD1	1.67	1.28
1:D:917:ILE:H	1:D:917:ILE:CD1	1.56	1.15
1:A:798:TRP:HB3	1:A:799:PRO:CD	1.76	1.15
1:A:744:LEU:HD22	1:A:798:TRP:NE1	1.60	1.13
1:D:917:ILE:HD13	1:D:917:ILE:N	1.56	1.11
1:A:259:LEU:HB3	1:A:767:MET:HE3	1.29	1.11
1:A:595:VAL:O	1:A:596:LEU:HB2	1.49	1.11
1:A:264:ILE:HG21	1:A:268:VAL:HG13	1.19	1.10
1:B:296:LEU:HB3	1:B:297:PRO:HD3	1.33	1.10
1:D:965:ILE:HG12	1:D:1125:GLU:HG2	1.26	1.10
1:D:312:THR:HG22	1:D:338:TRP:HE1	1.14	1.10
1:A:312:THR:HG22	1:A:338:TRP:HE1	1.11	1.09
1:A:798:TRP:HB3	1:A:799:PRO:HD3	1.12	1.07
1:C:917:ILE:H	1:C:917:ILE:CD1	1.60	1.07
1:C:917:ILE:H	1:C:917:ILE:HD13	0.92	1.07
1:D:182:MET:HE3	1:D:212:LEU:HB3	1.36	1.07
1:B:36:MET:HE3	1:B:83:MET:HG2	1.32	1.06
1:A:917:ILE:N	1:A:917:ILE:HD13	1.71	1.05
1:A:917:ILE:HD13	1:A:917:ILE:H	0.96	1.05
1:B:152:HIS:CD2	1:B:706:ILE:HB	1.93	1.03
1:B:706:ILE:HD13	1:B:706:ILE:N	1.73	1.03
1:A:259:LEU:HB3	1:A:767:MET:CE	1.88	1.01
1:B:264:ILE:HG21	1:B:268:VAL:HG13	1.37	1.01
1:D:276:ARG:HH12	1:D:326:GLU:HA	1.23	1.01
1:A:917:ILE:H	1:A:917:ILE:CD1	1.74	1.00
1:B:325:ASN:HD21	1:B:328:GLY:H	1.03	1.00
1:C:708:ARG:HB3	1:C:708:ARG:HH11	1.28	0.99
1:C:917:ILE:HD13	1:C:917:ILE:N	1.76	0.98
1:C:708:ARG:HB2	1:C:708:ARG:NH1	1.78	0.98
1:C:708:ARG:HH11	1:C:708:ARG:CB	1.76	0.98
1:B:1204:ASP:O	1:B:1221:ARG:NH1	1.97	0.97
1:B:534:THR:HG22	1:B:573:GLY:HA3	1.47	0.96
1:D:712:PRO:O	1:D:713:GLU:HB3	1.64	0.96
1:B:296:LEU:HB3	1:B:297:PRO:CD	1.96	0.95
1:A:798:TRP:CB	1:A:799:PRO:HD3	1.96	0.94
1:B:152:HIS:HA	1:B:706:ILE:HG13	1.49	0.94
1:A:185:ILE:O	1:A:189:ARG:HG2	1.67	0.94
1:C:708:ARG:NH1	1:C:708:ARG:CB	2.31	0.94
1:B:883:SER:HA	1:B:911:GLU:HG2	1.50	0.93
1:B:934:ALA:HB2	1:B:956:LYS:HD2	1.50	0.92
1:A:264:ILE:HG21	1:A:268:VAL:CG1	1.98	0.92
1:A:264:ILE:CG2	1:A:268:VAL:HG13	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:965:ILE:HG12	1:B:1125:GLU:HG2	1.49	0.92
1:D:917:ILE:H	1:D:917:ILE:HD13	0.74	0.91
1:A:312:THR:CG2	1:A:338:TRP:HE1	1.82	0.91
1:A:1092:THR:O	1:A:1093:VAL:HG22	1.68	0.91
1:D:159:THR:HA	1:D:162:GLN:HG3	1.51	0.91
1:D:312:THR:HG22	1:D:338:TRP:NE1	1.86	0.91
1:B:220:HIS:HE1	1:B:735:LEU:H	1.19	0.90
1:B:16:GLN:HE22	1:B:799:PRO:CG	1.85	0.90
1:C:1102:LYS:HB2	1:C:1103:PRO:HD3	1.55	0.89
1:A:461:SER:O	1:A:462:ILE:HG13	1.72	0.89
1:A:862:ILE:HD12	1:A:862:ILE:H	1.36	0.89
1:B:689:TYR:HB2	1:B:704:HIS:CD2	2.08	0.89
1:A:887:ASN:HD21	1:A:1195:LYS:HB2	1.36	0.88
1:A:982:THR:HB	1:A:983:GLN:HE21	1.35	0.88
1:A:534:THR:HG23	1:A:573:GLY:HA3	1.53	0.88
1:C:587:LYS:H	1:C:590:GLN:HE21	1.21	0.87
1:D:687:THR:O	1:D:704:HIS:HB3	1.75	0.87
1:A:312:THR:HG22	1:A:338:TRP:NE1	1.89	0.87
1:D:303:LYS:HE3	1:D:356:ASP:HA	1.55	0.87
1:C:264:ILE:CG2	1:C:268:VAL:HG13	2.04	0.87
1:D:292:PHE:CD1	1:D:544:VAL:HG22	2.10	0.87
1:C:219:HIS:HD2	1:C:254:ARG:HH11	1.18	0.86
1:D:1107:VAL:HG22	1:D:1108:SER:H	1.39	0.86
1:C:965:ILE:HG12	1:C:1125:GLU:HG2	1.57	0.86
1:B:58:GLU:O	1:B:62:SER:HB2	1.75	0.86
1:D:527:THR:HG22	1:D:528:ASP:H	1.39	0.86
1:A:744:LEU:CD2	1:A:798:TRP:CD1	2.57	0.85
1:C:220:HIS:HE1	1:C:735:LEU:H	1.24	0.85
1:A:132:ALA:O	1:A:137:THR:HG21	1.76	0.85
1:B:36:MET:CE	1:B:83:MET:HG2	2.05	0.85
1:B:595:VAL:O	1:B:596:LEU:HB2	1.77	0.85
1:C:342:LEU:HB3	1:C:567:ILE:HG21	1.57	0.84
1:A:534:THR:HG23	1:A:573:GLY:CA	2.07	0.84
1:D:418:PHE:HB3	1:D:455:PHE:HB2	1.60	0.84
1:B:155:ILE:HD11	1:B:166:VAL:HG21	1.57	0.84
1:B:531:LYS:HB3	1:B:531:LYS:NZ	1.93	0.84
1:A:309:LEU:O	1:A:312:THR:HB	1.78	0.83
1:D:135:PRO:HG2	1:D:591:GLN:HE22	1.41	0.83
1:A:1052:UNK:CB	1:A:1091:LYS:O	2.26	0.83
1:C:134:THR:O	1:C:140:MET:HG3	1.77	0.83
1:C:838:LYS:HG2	1:C:842:GLU:OE2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:LEU:O	1:A:534:THR:HB	1.78	0.82
1:B:592:LEU:O	1:B:595:VAL:O	1.97	0.82
1:C:969:ARG:HH21	1:C:972:LEU:HD22	1.44	0.82
1:C:398:LEU:HD13	1:C:442:LEU:HD21	1.60	0.82
1:D:152:HIS:CD2	1:D:706:ILE:HB	2.14	0.82
1:A:133:ILE:HA	1:A:140:MET:HE3	1.59	0.81
1:A:627:VAL:HG11	1:A:642:VAL:HG12	1.62	0.81
1:B:830:ARG:HG2	1:B:831:LYS:H	1.43	0.81
1:C:152:HIS:HD2	1:C:704:HIS:CE1	1.98	0.81
1:A:1196:ASN:ND2	1:A:1196:ASN:H	1.78	0.81
1:A:965:ILE:HG12	1:A:1125:GLU:HB3	1.61	0.81
1:A:1196:ASN:H	1:A:1196:ASN:HD22	1.28	0.81
1:B:945:ASN:ND2	1:B:1143:LYS:H	1.78	0.81
1:C:515:TYR:O	1:C:519:LYS:HG2	1.81	0.81
1:C:94:MET:HA	1:C:97:GLN:HE21	1.46	0.81
1:A:96:GLN:H	1:A:96:GLN:HE21	1.27	0.80
1:B:325:ASN:HD21	1:B:328:GLY:N	1.78	0.80
1:B:1114:LEU:HB3	1:B:1118:SER:HB3	1.61	0.80
1:B:325:ASN:ND2	1:B:328:GLY:H	1.78	0.80
1:C:132:ALA:O	1:C:137:THR:HG21	1.80	0.80
1:C:152:HIS:HA	1:C:706:ILE:HG12	1.64	0.80
1:A:595:VAL:O	1:A:596:LEU:CB	2.30	0.79
1:B:918:ASN:HD21	1:D:452:LEU:HD13	1.45	0.79
1:B:1115:THR:OG1	1:B:1118:SER:HB2	1.81	0.79
1:C:969:ARG:HH21	1:C:972:LEU:CD2	1.95	0.79
1:B:16:GLN:HE22	1:B:799:PRO:HG3	1.47	0.79
1:A:621:ASP:O	1:A:622:PHE:HB2	1.83	0.79
1:C:938:GLU:HB2	1:C:1182:HIS:NE2	1.98	0.79
1:A:366:ASN:O	1:A:370:GLU:HG3	1.83	0.79
1:A:687:THR:O	1:A:704:HIS:HB3	1.83	0.78
1:B:1216:ARG:O	1:B:1216:ARG:HG3	1.83	0.78
1:D:220:HIS:HE1	1:D:735:LEU:H	1.28	0.78
1:C:1038:UNK:O	1:C:1039:UNK:CB	2.32	0.78
1:A:864:ALA:HB3	1:A:895:LEU:HD12	1.65	0.78
1:D:299:LEU:HD22	1:D:309:LEU:HD11	1.64	0.78
1:B:220:HIS:CE1	1:B:735:LEU:H	2.02	0.77
1:C:961:ALA:O	1:C:1129:TYR:OH	2.01	0.77
1:D:1175:ASP:O	1:D:1175:ASP:OD1	2.03	0.77
1:C:701:GLU:O	1:C:703:ASN:N	2.13	0.77
1:B:91:ARG:HA	1:B:94:MET:HG2	1.65	0.77
1:D:152:HIS:HD2	1:D:706:ILE:HB	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:595:VAL:O	1:D:596:LEU:HB3	1.84	0.77
1:B:872:ASN:HD22	1:B:887:ASN:HD22	1.33	0.76
1:C:534:THR:HG22	1:C:573:GLY:HA3	1.68	0.76
1:D:91:ARG:HA	1:D:94:MET:HG2	1.66	0.76
1:D:574:ILE:O	1:D:574:ILE:HD12	1.85	0.76
1:C:219:HIS:HD2	1:C:254:ARG:NH1	1.82	0.76
1:A:36:MET:HG3	1:A:39:ILE:HD12	1.68	0.76
1:C:736:ALA:H	1:C:904:ASN:HD22	1.33	0.76
1:D:105:ALA:HB1	1:D:599:ARG:HD2	1.66	0.76
1:D:195:ASN:HD22	1:D:196:PRO:HD2	1.51	0.76
1:B:264:ILE:HG22	1:B:265:THR:N	2.01	0.76
1:B:739:PRO:HG3	1:B:800:PHE:CE2	2.20	0.76
1:D:729:LYS:NZ	1:D:904:ASN:HD21	1.84	0.75
1:C:155:ILE:HB	1:C:706:ILE:HG13	1.69	0.75
1:D:1235:ASP:O	1:D:1237:GLN:HG3	1.87	0.75
1:D:850:ASN:O	1:D:854:THR:HB	1.87	0.75
1:C:155:ILE:HB	1:C:706:ILE:CG1	2.15	0.75
1:C:840:PHE:HD2	1:C:841:ARG:HE	1.35	0.75
1:C:101:ARG:NH1	1:C:134:THR:OG1	2.19	0.74
1:B:98:ARG:HG2	1:B:595:VAL:HA	1.69	0.74
1:B:960:ARG:NH2	1:B:1133:PRO:O	2.17	0.74
1:B:917:ILE:HD13	1:B:917:ILE:H	1.51	0.74
1:D:266:ASP:O	1:D:267:SER:HB3	1.86	0.74
1:D:706:ILE:HD13	1:D:706:ILE:N	2.02	0.74
1:B:534:THR:HG22	1:B:573:GLY:CA	2.17	0.74
1:A:534:THR:CG2	1:A:573:GLY:CA	2.65	0.74
1:D:155:ILE:HB	1:D:706:ILE:HG13	1.70	0.74
1:A:7:PHE:O	1:A:10:ILE:HG22	1.87	0.74
1:A:963:PRO:HD3	1:A:1129:TYR:CZ	2.22	0.74
1:A:1204:ASP:O	1:A:1221:ARG:NH1	2.20	0.74
1:D:962:GLU:HG3	1:D:1169:ARG:HE	1.53	0.74
1:A:543:TRP:CD1	1:A:553:PRO:HG2	2.23	0.73
1:C:98:ARG:NH1	1:C:645:SER:O	2.21	0.73
1:B:264:ILE:CG2	1:B:268:VAL:HG13	2.18	0.73
1:C:958:SER:HB2	1:C:1134:ASP:OD1	1.87	0.73
1:A:1232:ASN:C	1:A:1232:ASN:HD22	1.92	0.73
1:C:768:VAL:HG11	1:C:858:LEU:HD22	1.71	0.73
1:D:91:ARG:HA	1:D:94:MET:CG	2.18	0.73
1:D:676:ASP:HB2	1:D:711:ILE:HG22	1.70	0.73
1:A:826:LYS:HG3	1:A:827:VAL:N	2.03	0.73
1:B:16:GLN:NE2	1:B:799:PRO:HG2	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:HIS:HD2	1:B:704:HIS:CE1	2.06	0.73
1:D:334:ARG:HA	1:D:337:ILE:HD12	1.71	0.73
1:A:826:LYS:HG3	1:A:827:VAL:H	1.53	0.73
1:B:54:ARG:HD2	1:B:128:PHE:N	2.04	0.73
1:C:539:GLY:HA2	1:C:578:ILE:HD13	1.70	0.73
1:B:16:GLN:HE22	1:B:799:PRO:HG2	1.53	0.72
1:B:665:PRO:HA	1:B:668:LYS:HB2	1.71	0.72
1:D:691:THR:HG22	1:D:699:ASP:OD2	1.89	0.72
1:D:969:ARG:HD2	1:D:1121:ALA:HB3	1.70	0.72
1:B:1137:GLU:HG2	1:B:1138:GLN:H	1.53	0.72
1:A:606:VAL:O	1:A:607:VAL:HG23	1.89	0.72
1:D:33:TYR:OH	1:D:200:HIS:HD2	1.72	0.72
1:C:33:TYR:OH	1:C:200:HIS:HD2	1.71	0.72
1:C:815:VAL:HG11	1:C:830:ARG:NH1	2.04	0.72
1:D:395:LYS:HB3	1:D:396:PRO:CD	2.19	0.72
1:B:706:ILE:N	1:B:706:ILE:CD1	2.49	0.72
1:D:152:HIS:HE1	1:D:708:ARG:HE	1.38	0.72
1:B:298:ASP:HB3	1:B:300:HIS:HE1	1.55	0.72
1:C:883:SER:HA	1:C:911:GLU:HG2	1.71	0.72
1:D:299:LEU:HD22	1:D:309:LEU:CD1	2.19	0.72
1:B:1145:PRO:HB2	1:B:1147:GLU:OE1	1.89	0.71
1:D:137:THR:HG22	1:D:138:GLU:H	1.54	0.71
1:D:952:LEU:HD11	1:D:1144:VAL:HG21	1.72	0.71
1:D:292:PHE:HD1	1:D:544:VAL:HG22	1.55	0.71
1:B:798:TRP:O	1:B:799:PRO:C	2.27	0.71
1:C:707:GLU:N	1:C:707:GLU:OE1	2.24	0.71
1:D:276:ARG:NH1	1:D:326:GLU:HA	2.02	0.70
1:D:395:LYS:HB3	1:D:396:PRO:HD3	1.72	0.70
1:A:156:THR:HG23	1:A:703:ASN:O	1.91	0.70
1:A:1189:GLY:O	1:A:1200:GLN:HB2	1.92	0.70
1:C:152:HIS:CE1	1:C:708:ARG:HG2	2.26	0.70
1:D:705:CYS:C	1:D:706:ILE:HD13	2.10	0.70
1:A:952:LEU:HD13	1:A:1149:ILE:HD11	1.74	0.70
1:B:830:ARG:HG2	1:B:831:LYS:N	2.06	0.70
1:C:137:THR:HG22	1:C:140:MET:H	1.55	0.69
1:A:264:ILE:O	1:A:266:ASP:N	2.25	0.69
1:C:688:VAL:HG13	1:C:701:GLU:HA	1.73	0.69
1:D:756:VAL:HG23	1:D:853:ARG:HG2	1.73	0.69
1:A:1237:GLN:O	1:A:1238:LEU:HD23	1.91	0.69
1:B:195:ASN:ND2	1:B:197:ASN:H	1.89	0.69
1:B:531:LYS:HB3	1:B:531:LYS:HZ3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:ASN:ND2	1:A:1143:LYS:H	1.90	0.69
1:C:220:HIS:CE1	1:C:735:LEU:H	2.10	0.69
1:A:729:LYS:HB3	1:A:733:SER:O	1.93	0.69
1:B:946:SER:OG	1:B:947:GLU:N	2.26	0.69
1:C:212:LEU:HD21	1:C:548:TYR:CD1	2.27	0.69
1:C:514:GLN:NE2	1:C:517:LYS:HD2	2.08	0.69
1:B:626:GLU:O	1:B:627:VAL:HG23	1.92	0.69
1:D:1107:VAL:HG13	1:D:1108:SER:O	1.93	0.69
1:A:96:GLN:HE21	1:A:96:GLN:N	1.91	0.68
1:D:146:ASN:O	1:D:149:TYR:HB3	1.94	0.68
1:A:706:ILE:N	1:A:706:ILE:HD12	2.09	0.68
1:B:928:VAL:HG21	1:B:1173:ILE:HG22	1.74	0.68
1:B:945:ASN:HD22	1:B:1143:LYS:H	1.40	0.68
1:B:417:ILE:HG13	1:B:454:TYR:CD1	2.29	0.68
1:D:221:PHE:HB3	1:D:250:LEU:HD12	1.74	0.68
1:B:312:THR:HG22	1:B:338:TRP:HE1	1.56	0.68
1:A:58:GLU:HG3	1:A:59:GLU:N	2.07	0.68
1:B:963:PRO:HD3	1:B:1129:TYR:CZ	2.28	0.68
1:C:1234:SER:O	1:C:1235:ASP:HB3	1.92	0.68
1:A:461:SER:C	1:A:462:ILE:HG13	2.13	0.68
1:B:705:CYS:C	1:B:706:ILE:HD13	2.13	0.68
1:A:982:THR:HB	1:A:983:GLN:NE2	2.09	0.68
1:B:16:GLN:NE2	1:B:799:PRO:CG	2.57	0.68
1:C:256:TYR:HA	1:C:259:LEU:HD12	1.75	0.68
1:D:391:ILE:HG22	1:D:436:PHE:HE1	1.59	0.68
1:B:917:ILE:HG13	1:B:947:GLU:O	1.93	0.67
1:C:516:TYR:CE2	1:C:533:MET:HE1	2.30	0.67
1:C:706:ILE:N	1:C:706:ILE:HD12	2.10	0.67
1:B:300:HIS:HB2	1:B:360:PHE:CZ	2.29	0.67
1:B:917:ILE:HD13	1:B:917:ILE:N	2.09	0.67
1:C:264:ILE:HG21	1:C:268:VAL:HG13	1.76	0.67
1:C:1160:ARG:HG3	1:C:1227:SER:OG	1.94	0.67
1:A:55:LEU:HD12	1:A:55:LEU:H	1.60	0.67
1:D:391:ILE:HG22	1:D:436:PHE:CE1	2.30	0.67
1:B:199:ARG:HG2	1:B:738:PHE:CZ	2.30	0.67
1:C:862:ILE:HD12	1:C:862:ILE:H	1.59	0.67
1:A:797:ARG:O	1:A:798:TRP:C	2.33	0.67
1:C:152:HIS:HE1	1:C:708:ARG:HG2	1.58	0.67
1:C:1213:PHE:O	1:C:1216:ARG:NH1	2.27	0.67
1:A:1093:VAL:HB	1:A:1094:ALA:HA	1.76	0.67
1:A:928:VAL:HG21	1:A:1173:ILE:HG23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LYS:HZ2	1:B:357:VAL:HG23	1.60	0.66
1:B:918:ASN:ND2	1:D:452:LEU:HD13	2.09	0.66
1:D:807:LEU:HD11	1:D:869:VAL:HG13	1.76	0.66
1:D:1138:GLN:O	1:D:1138:GLN:HG2	1.93	0.66
1:A:262:GLU:O	1:A:264:ILE:N	2.28	0.66
1:A:199:ARG:HD3	1:A:735:LEU:HD23	1.76	0.66
1:A:627:VAL:HG11	1:A:642:VAL:CG1	2.25	0.66
1:B:566:ARG:O	1:B:570:VAL:HG23	1.95	0.66
1:B:219:HIS:HD2	1:B:254:ARG:HE	1.43	0.66
1:D:156:THR:N	1:D:706:ILE:HD11	2.10	0.66
1:A:712:PRO:O	1:A:713:GLU:CB	2.44	0.66
1:D:676:ASP:HB2	1:D:711:ILE:CG2	2.25	0.66
1:C:152:HIS:O	1:C:706:ILE:CD1	2.44	0.66
1:D:171:HIS:CE1	1:D:172:GLU:OE2	2.49	0.66
1:D:195:ASN:HB3	1:D:198:THR:OG1	1.96	0.66
1:A:648:ASP:OD1	1:A:651:ARG:HB2	1.96	0.65
1:A:320:MET:HE3	1:A:322:GLY:O	1.96	0.65
1:A:1232:ASN:HD22	1:A:1233:LEU:N	1.95	0.65
1:B:303:LYS:NZ	1:B:357:VAL:HG23	2.11	0.65
1:A:826:LYS:CG	1:A:827:VAL:H	2.10	0.65
1:A:254:ARG:HH22	1:A:724:LEU:HD21	1.60	0.65
1:A:786:ALA:O	1:A:790:MET:HB2	1.97	0.65
1:C:840:PHE:O	1:C:844:LYS:HB2	1.97	0.65
1:D:746:LEU:CD1	1:D:769:LEU:HD22	2.26	0.65
1:C:312:THR:HG22	1:C:338:TRP:NE1	2.12	0.65
1:C:312:THR:HG22	1:C:338:TRP:CD1	2.31	0.65
1:D:512:LYS:O	1:D:516:TYR:CD1	2.49	0.65
1:D:701:GLU:C	1:D:703:ASN:H	2.00	0.65
1:D:712:PRO:O	1:D:713:GLU:CB	2.43	0.65
1:B:335:PHE:O	1:B:335:PHE:CD1	2.50	0.65
1:B:837:ARG:O	1:B:841:ARG:HG2	1.97	0.65
1:B:159:THR:OG1	1:B:1175:ASP:HB3	1.95	0.65
1:B:290:ASN:N	1:B:290:ASN:ND2	2.44	0.65
1:D:357:VAL:HG12	1:D:361:ASN:HD21	1.61	0.65
1:A:584:GLN:HG2	1:A:585:PRO:HD2	1.79	0.65
1:B:152:HIS:HA	1:B:706:ILE:CG1	2.26	0.64
1:C:96:GLN:NE2	1:C:100:ARG:HH21	1.95	0.64
1:C:708:ARG:HB2	1:C:708:ARG:CZ	2.27	0.64
1:D:330:ILE:HD12	1:D:542:GLN:HG2	1.78	0.64
1:D:729:LYS:HZ3	1:D:904:ASN:HD21	1.43	0.64
1:A:250:LEU:O	1:A:254:ARG:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:THR:HG22	1:B:699:ASP:OD1	1.97	0.64
1:C:768:VAL:CG1	1:C:858:LEU:HD22	2.27	0.64
1:D:945:ASN:ND2	1:D:1143:LYS:H	1.96	0.64
1:B:298:ASP:HB3	1:B:300:HIS:CE1	2.33	0.64
1:C:837:ARG:HD3	1:C:841:ARG:HH22	1.62	0.64
1:C:1086:ALA:HA	1:C:1089:ILE:HD12	1.80	0.64
1:C:248:LEU:HD23	1:C:249:HIS:N	2.12	0.64
1:C:264:ILE:HG23	1:C:268:VAL:HG13	1.79	0.64
1:A:155:ILE:HB	1:A:706:ILE:CG1	2.28	0.64
1:D:91:ARG:HG2	1:D:558:TYR:HB3	1.78	0.64
1:C:290:ASN:HD22	1:C:292:PHE:H	1.46	0.64
1:D:340:LYS:HZ2	1:D:340:LYS:HA	1.63	0.64
1:B:278:LEU:O	1:B:282:ILE:HD12	1.98	0.63
1:B:676:ASP:HB3	1:B:711:ILE:HG22	1.80	0.63
1:B:312:THR:HG23	1:B:341:TYR:HB3	1.80	0.63
1:B:933:TYR:CE1	1:B:956:LYS:HD3	2.33	0.63
1:C:691:THR:HG22	1:C:699:ASP:OD1	1.98	0.63
1:C:1204:ASP:O	1:C:1221:ARG:NH1	2.32	0.63
1:D:25:GLN:NE2	1:D:906:ASP:OD2	2.32	0.63
1:A:156:THR:CG2	1:A:703:ASN:O	2.47	0.63
1:B:290:ASN:N	1:B:290:ASN:HD22	1.95	0.63
1:B:533:MET:HA	1:B:561:TYR:CE2	2.34	0.63
1:C:815:VAL:HG11	1:C:830:ARG:HH11	1.62	0.63
1:A:802:ARG:HD2	1:A:870:PRO:HB2	1.80	0.63
1:A:922:PRO:O	1:A:925:SER:HB3	1.97	0.63
1:B:965:ILE:HD12	1:B:966:GLY:H	1.62	0.63
1:C:156:THR:N	1:C:706:ILE:HD11	2.13	0.63
1:D:312:THR:HG21	1:D:342:LEU:HD23	1.80	0.63
1:B:403:GLN:O	1:B:404:ARG:HB2	1.97	0.62
1:C:111:ALA:O	1:C:113:GLN:N	2.31	0.62
1:C:155:ILE:CG2	1:C:706:ILE:HG13	2.28	0.62
1:C:219:HIS:CD2	1:C:254:ARG:HH11	2.09	0.62
1:C:729:LYS:HD2	1:C:735:LEU:HD13	1.81	0.62
1:D:701:GLU:C	1:D:703:ASN:N	2.51	0.62
1:A:93:LYS:O	1:A:96:GLN:HG2	1.98	0.62
1:A:111:ALA:O	1:A:112:LEU:C	2.37	0.62
1:A:793:ILE:O	1:A:793:ILE:HG22	1.97	0.62
1:D:317:LEU:HA	1:D:320:MET:HE1	1.82	0.62
1:D:957:GLY:HA2	1:D:1136:SER:HB2	1.80	0.62
1:A:58:GLU:OE1	1:A:695:GLY:HA3	1.99	0.62
1:B:881:SER:HB3	1:B:914:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:ILE:HB	1:A:1196:ASN:OD1	2.00	0.62
1:B:155:ILE:CG2	1:B:706:ILE:HD12	2.30	0.62
1:B:622:PHE:HD2	1:B:622:PHE:O	1.83	0.62
1:D:595:VAL:O	1:D:596:LEU:CB	2.47	0.62
1:D:746:LEU:HD11	1:D:769:LEU:HD22	1.80	0.62
1:A:155:ILE:HB	1:A:706:ILE:HG13	1.80	0.62
1:A:219:HIS:CE1	1:A:251:SER:HB2	2.34	0.62
1:B:1182:HIS:O	1:B:1183:SER:C	2.37	0.62
1:D:33:TYR:OH	1:D:200:HIS:CD2	2.52	0.62
1:A:535:GLU:HG2	1:A:576:GLN:CD	2.20	0.62
1:B:423:LYS:O	1:B:427:ARG:HG2	2.00	0.62
1:C:831:LYS:O	1:C:833:GLN:N	2.26	0.62
1:B:443:ILE:HG13	1:B:458:ASP:HB2	1.81	0.62
1:C:1102:LYS:CB	1:C:1103:PRO:HD3	2.26	0.62
1:C:949:ARG:HE	1:C:1145:PRO:HB3	1.65	0.62
1:A:593:MET:HE2	1:A:604:ILE:HD13	1.82	0.62
1:A:798:TRP:O	1:A:799:PRO:C	2.37	0.62
1:A:820:LYS:HA	1:A:825:THR:HG22	1.82	0.62
1:C:325:ASN:HD21	1:C:328:GLY:H	1.47	0.62
1:D:512:LYS:O	1:D:516:TYR:HD1	1.82	0.62
1:D:965:ILE:CG1	1:D:1125:GLU:HG2	2.16	0.61
1:A:862:ILE:HD12	1:A:862:ILE:N	2.13	0.61
1:C:309:LEU:O	1:C:312:THR:HB	1.99	0.61
1:B:312:THR:HG22	1:B:338:TRP:NE1	2.14	0.61
1:C:91:ARG:HA	1:C:94:MET:HG3	1.83	0.61
1:C:307:PRO:HG2	1:C:764:GLN:HG2	1.81	0.61
1:D:22:ASP:OD2	1:D:24:SER:HB3	2.01	0.61
1:D:879:ASP:OD1	1:D:879:ASP:N	2.32	0.61
1:A:152:HIS:HD2	1:A:704:HIS:NE2	1.98	0.61
1:D:945:ASN:OD1	1:D:951:LYS:HD2	2.00	0.61
1:A:701:GLU:O	1:A:704:HIS:N	2.34	0.61
1:B:981:PRO:HB3	1:B:1037:UNK:CB	2.31	0.61
1:D:325:ASN:HD21	1:D:328:GLY:CA	2.14	0.61
1:D:390:LEU:HD11	1:D:455:PHE:HE1	1.66	0.61
1:C:97:GLN:O	1:C:101:ARG:HB2	2.01	0.61
1:A:962:GLU:HG3	1:A:1169:ARG:HE	1.66	0.61
1:B:601:LYS:O	1:B:604:ILE:HD11	2.01	0.61
1:C:228:VAL:HG12	1:C:228:VAL:O	2.01	0.61
1:D:1232:ASN:C	1:D:1232:ASN:HD22	2.03	0.61
1:A:876:ARG:NH1	1:A:920:GLU:OE2	2.34	0.60
1:A:955:LYS:HG3	1:A:1138:GLN:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:ILE:HA	1:A:1220:ARG:HH12	1.65	0.60
1:D:929:PHE:HD1	1:D:1149:ILE:CD1	2.14	0.60
1:A:259:LEU:CB	1:A:767:MET:CE	2.72	0.60
1:A:307:PRO:HG2	1:A:764:GLN:HG2	1.82	0.60
1:B:601:LYS:O	1:B:604:ILE:CD1	2.49	0.60
1:B:785:LEU:HD23	1:B:789:HIS:HD2	1.66	0.60
1:B:1181:LEU:O	1:B:1182:HIS:HB2	2.00	0.60
1:C:16:GLN:NE2	1:C:799:PRO:HG3	2.16	0.60
1:C:770:HIS:CE1	1:C:858:LEU:HD23	2.37	0.60
1:C:1232:ASN:ND2	1:C:1234:SER:O	2.35	0.60
1:D:701:GLU:O	1:D:703:ASN:N	2.34	0.60
1:D:948:THR:HG22	1:D:1146:ARG:NH2	2.15	0.60
1:C:917:ILE:CD1	1:C:947:GLU:O	2.49	0.60
1:D:534:THR:HG22	1:D:573:GLY:HA3	1.82	0.60
1:B:918:ASN:H	1:B:918:ASN:HD22	1.48	0.60
1:B:1193:ILE:CG2	1:B:1193:ILE:O	2.49	0.60
1:C:152:HIS:O	1:C:706:ILE:HD13	2.01	0.60
1:C:312:THR:HG22	1:C:338:TRP:HE1	1.64	0.60
1:C:706:ILE:HG22	1:C:707:GLU:N	2.16	0.60
1:D:210:ILE:HA	1:D:223:LEU:CD1	2.32	0.60
1:A:416:GLU:HB2	1:C:951:LYS:NZ	2.17	0.60
1:B:595:VAL:O	1:B:596:LEU:CB	2.48	0.60
1:C:949:ARG:HD3	1:C:1143:LYS:O	2.01	0.60
1:C:1181:LEU:O	1:C:1182:HIS:HB2	2.00	0.60
1:A:969:ARG:NH1	1:A:972:LEU:HD23	2.17	0.60
1:A:1212:ASN:ND2	1:A:1215:GLY:H	2.00	0.60
1:B:512:LYS:HD2	1:B:566:ARG:HG3	1.83	0.60
1:B:182:MET:HE3	1:B:182:MET:HA	1.84	0.60
1:C:393:ALA:HB1	1:C:418:PHE:HZ	1.67	0.60
1:A:209:LEU:HD23	1:A:212:LEU:HD12	1.83	0.59
1:D:928:VAL:HG21	1:D:1173:ILE:HG22	1.84	0.59
1:C:1189:GLY:O	1:C:1200:GLN:HB2	2.02	0.59
1:B:300:HIS:HB2	1:B:360:PHE:HZ	1.67	0.59
1:A:312:THR:CG2	1:A:338:TRP:NE1	2.54	0.59
1:A:794:VAL:HG22	1:A:804:SER:O	2.02	0.59
1:A:798:TRP:CE3	1:A:799:PRO:HD3	2.38	0.59
1:B:152:HIS:CD2	1:B:704:HIS:CE1	2.90	0.59
1:C:1169:ARG:HH11	1:C:1186:THR:HG23	1.68	0.59
1:D:3:ILE:HB	1:D:6:PHE:HB2	1.84	0.59
1:D:251:SER:O	1:D:255:GLU:HG3	2.01	0.59
1:D:264:ILE:HG22	1:D:265:THR:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:LYS:HD2	1:A:831:LYS:H	1.66	0.59
1:B:36:MET:HE2	1:B:68:ILE:HG12	1.84	0.59
1:C:701:GLU:C	1:C:703:ASN:H	2.05	0.59
1:D:159:THR:CA	1:D:162:GLN:HG3	2.31	0.59
1:D:312:THR:CG2	1:D:338:TRP:NE1	2.63	0.59
1:D:744:LEU:HD21	1:D:897:LEU:HA	1.85	0.59
1:B:1147:GLU:CD	1:B:1147:GLU:H	2.06	0.59
1:B:1224:GLY:O	1:B:1225:LEU:HD23	2.03	0.59
1:C:873:GLY:HA2	1:C:909:TYR:HE2	1.66	0.59
1:A:304:GLY:O	1:A:307:PRO:HD2	2.03	0.59
1:B:96:GLN:NE2	1:B:100:ARG:HH21	2.01	0.59
1:D:747:THR:HG22	1:D:770:HIS:HB2	1.84	0.59
1:A:325:ASN:HD21	1:A:328:GLY:CA	2.15	0.59
1:A:751:ALA:O	1:A:765:GLN:HA	2.03	0.58
1:B:10:ILE:HG12	1:B:14:TRP:CZ3	2.38	0.58
1:B:950:LEU:HD23	1:B:1144:VAL:O	2.03	0.58
1:D:220:HIS:CE1	1:D:735:LEU:H	2.16	0.58
1:B:315:GLU:HB3	1:B:341:TYR:CZ	2.38	0.58
1:B:965:ILE:CG1	1:B:1125:GLU:HG2	2.28	0.58
1:C:219:HIS:CE1	1:C:251:SER:HB2	2.38	0.58
1:C:300:HIS:HB3	1:C:303:LYS:HB2	1.83	0.58
1:C:155:ILE:CB	1:C:706:ILE:HG13	2.33	0.58
1:D:687:THR:O	1:D:704:HIS:CB	2.50	0.58
1:D:6:PHE:CZ	1:D:10:ILE:HD12	2.39	0.58
1:A:1093:VAL:CB	1:A:1094:ALA:HA	2.32	0.58
1:A:91:ARG:O	1:A:93:LYS:N	2.35	0.58
1:A:593:MET:CE	1:A:604:ILE:HD13	2.34	0.58
1:A:744:LEU:HD21	1:A:897:LEU:HA	1.85	0.58
1:D:181:ILE:O	1:D:185:ILE:HG13	2.04	0.58
1:B:602:ASN:OD1	1:B:602:ASN:N	2.36	0.58
1:B:774:LEU:HD12	1:B:774:LEU:H	1.68	0.58
1:A:854:THR:HG22	1:A:855:LYS:HG2	1.86	0.58
1:A:1193:ILE:H	1:A:1193:ILE:HD12	1.67	0.58
1:C:175:GLY:O	1:C:180:LYS:HE2	2.04	0.58
1:A:927:VAL:HG23	1:A:939:ALA:HB3	1.85	0.58
1:A:744:LEU:CD2	1:A:798:TRP:NE1	2.52	0.57
1:B:949:ARG:HH11	1:B:949:ARG:HG2	1.68	0.57
1:D:137:THR:HG22	1:D:138:GLU:N	2.18	0.57
1:D:313:PHE:CE1	1:D:317:LEU:HD13	2.39	0.57
1:D:342:LEU:O	1:D:345:PHE:HB3	2.04	0.57
1:D:664:SER:HB2	1:D:667:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLU:OE1	1:A:369:LEU:HG	2.04	0.57
1:C:359:TRP:CZ2	1:C:363:GLN:NE2	2.72	0.57
1:A:446:HIS:CE1	1:A:450:LYS:HE3	2.39	0.57
1:B:965:ILE:HG12	1:B:1125:GLU:CG	2.30	0.57
1:C:1084:ALA:O	1:C:1085:GLU:C	2.43	0.57
1:D:339:LEU:HD11	1:D:570:VAL:HB	1.86	0.57
1:D:262:GLU:HG2	1:D:263:GLU:N	2.19	0.57
1:D:335:PHE:O	1:D:339:LEU:HB2	2.04	0.57
1:D:527:THR:HG22	1:D:528:ASP:N	2.13	0.57
1:D:704:HIS:ND1	1:D:705:CYS:N	2.53	0.57
1:D:965:ILE:HG12	1:D:1125:GLU:CG	2.19	0.57
1:A:407:THR:HG22	1:A:408:SER:H	1.68	0.57
1:D:387:GLN:HG2	1:D:432:PHE:CZ	2.40	0.57
1:A:592:LEU:O	1:A:595:VAL:O	2.23	0.57
1:B:588:PRO:HD2	1:B:671:ASN:O	2.04	0.57
1:D:676:ASP:CB	1:D:711:ILE:HG22	2.35	0.57
1:C:165:LYS:NZ	1:C:165:LYS:CB	2.68	0.57
1:D:412:ASP:HB2	1:D:459:LEU:HD22	1.87	0.57
1:A:811:THR:HG22	1:A:813:GLU:H	1.70	0.57
1:B:516:TYR:CE2	1:B:533:MET:HE2	2.39	0.57
1:D:10:ILE:HD13	1:D:14:TRP:HZ3	1.69	0.57
1:D:933:TYR:CE1	1:D:1139:LYS:HE2	2.39	0.57
1:B:155:ILE:HG22	1:B:706:ILE:HD12	1.86	0.56
1:B:264:ILE:O	1:B:266:ASP:N	2.36	0.56
1:C:540:GLY:HA2	1:C:557:TRP:CZ2	2.40	0.56
1:C:593:MET:HB3	1:C:652:LEU:HD11	1.86	0.56
1:B:627:VAL:HG11	1:B:643:LYS:CB	2.35	0.56
1:C:135:PRO:HB3	1:C:171:HIS:HB2	1.87	0.56
1:D:917:ILE:HD12	1:D:947:GLU:O	2.06	0.56
1:B:689:TYR:HB3	1:B:700:ILE:HD12	1.86	0.56
1:B:182:MET:HA	1:B:182:MET:CE	2.35	0.56
1:B:789:HIS:O	1:B:792:LYS:HB2	2.05	0.56
1:D:292:PHE:HD1	1:D:544:VAL:CG2	2.18	0.56
1:A:918:ASN:HD22	1:A:918:ASN:H	1.54	0.56
1:D:16:GLN:HE21	1:D:855:LYS:HD2	1.69	0.56
1:A:194:TYR:OH	1:A:200:HIS:HE1	1.88	0.56
1:C:974:SER:HB3	1:C:975:GLN:NE2	2.21	0.56
1:D:715:MET:O	1:D:716:GLU:CB	2.53	0.56
1:B:28:GLU:O	1:B:199:ARG:HD2	2.05	0.56
1:D:830:ARG:NH1	1:D:836:GLU:OE2	2.38	0.56
1:D:938:GLU:HB2	1:D:1182:HIS:NE2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:VAL:HG12	1:B:642:VAL:H	1.71	0.56
1:C:512:LYS:C	1:C:514:GLN:H	2.09	0.56
1:D:531:LYS:O	1:D:535:GLU:HG3	2.05	0.56
1:D:1171:MET:HB3	1:D:1173:ILE:HD11	1.88	0.56
1:A:798:TRP:CB	1:A:799:PRO:CD	2.48	0.55
1:B:342:LEU:O	1:B:345:PHE:HB3	2.05	0.55
1:B:649:GLN:O	1:B:653:VAL:HG23	2.05	0.55
1:C:514:GLN:O	1:C:517:LYS:HB3	2.06	0.55
1:A:98:ARG:NH1	1:A:644:ILE:HG12	2.21	0.55
1:A:264:ILE:HG22	1:A:265:THR:N	2.20	0.55
1:D:893:TYR:HB2	1:D:898:ILE:HD11	1.89	0.55
1:D:173:VAL:HG21	1:D:676:ASP:OD1	2.07	0.55
1:D:969:ARG:HD2	1:D:1121:ALA:CB	2.35	0.55
1:D:1192:SER:HB3	1:D:1197:VAL:HG13	1.88	0.55
1:A:301:LEU:C	1:A:303:LYS:H	2.09	0.55
1:B:185:ILE:O	1:B:189:ARG:HG2	2.06	0.55
1:C:833:GLN:O	1:C:833:GLN:HG3	2.06	0.55
1:D:679:PHE:CD1	1:D:679:PHE:N	2.73	0.55
1:D:969:ARG:HD3	1:D:1118:SER:HA	1.88	0.55
1:A:505:SER:HB3	1:A:508:PHE:HB2	1.88	0.55
1:A:1232:ASN:C	1:A:1232:ASN:ND2	2.57	0.55
1:B:152:HIS:CD2	1:B:704:HIS:NE2	2.75	0.55
1:B:1105:VAL:HG12	1:B:1105:VAL:O	2.07	0.55
1:C:401:THR:HG22	1:C:457:LEU:HD22	1.87	0.55
1:C:446:HIS:HD2	1:C:447:SER:O	1.90	0.55
1:C:798:TRP:O	1:C:799:PRO:C	2.45	0.55
1:A:700:ILE:HG22	1:A:704:HIS:HB2	1.89	0.55
1:B:155:ILE:O	1:B:162:GLN:NE2	2.40	0.55
1:A:102:PHE:HA	1:A:597:PRO:HG3	1.88	0.55
1:A:262:GLU:HG3	1:A:263:GLU:N	2.21	0.55
1:A:701:GLU:O	1:A:703:ASN:N	2.40	0.55
1:A:844:LYS:HB2	1:A:862:ILE:HD13	1.87	0.55
1:C:713:GLU:HG2	1:C:715:MET:H	1.71	0.55
1:A:158:ASP:OD1	1:A:1176:SER:HB2	2.07	0.55
1:A:292:PHE:N	1:A:292:PHE:CD1	2.75	0.55
1:A:887:ASN:HD21	1:A:1195:LYS:CB	2.13	0.55
1:D:1118:SER:O	1:D:1122:VAL:HG23	2.07	0.55
1:A:1093:VAL:HB	1:A:1094:ALA:CA	2.36	0.54
1:C:307:PRO:CG	1:C:764:GLN:HG2	2.37	0.54
1:C:1189:GLY:O	1:C:1200:GLN:CB	2.55	0.54
1:D:756:VAL:CG2	1:D:853:ARG:HG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1107:VAL:HG22	1:D:1108:SER:N	2.17	0.54
1:C:312:THR:HG23	1:C:341:TYR:HB2	1.88	0.54
1:D:946:SER:HB3	1:D:948:THR:H	1.73	0.54
1:A:945:ASN:HD21	1:A:951:LYS:HB3	1.73	0.54
1:C:376:THR:C	1:C:378:MET:H	2.09	0.54
1:A:315:GLU:O	1:A:319:HIS:HD2	1.91	0.54
1:A:512:LYS:HG2	1:A:566:ARG:HG3	1.89	0.54
1:A:850:ASN:O	1:A:854:THR:HB	2.08	0.54
1:B:330:ILE:N	1:B:542:GLN:OE1	2.36	0.54
1:C:1111:SER:CB	1:C:1191:THR:HA	2.37	0.54
1:D:786:ALA:O	1:D:790:MET:HB2	2.07	0.54
1:A:589:PHE:CE2	1:A:671:ASN:HB2	2.43	0.54
1:C:512:LYS:O	1:C:514:GLN:N	2.31	0.54
1:D:867:LYS:HG3	1:D:892:TYR:CE2	2.42	0.54
1:A:91:ARG:C	1:A:93:LYS:H	2.11	0.54
1:A:407:THR:HG22	1:A:408:SER:N	2.22	0.54
1:B:100:ARG:NH1	1:B:101:ARG:HH12	2.06	0.54
1:B:933:TYR:CZ	1:B:956:LYS:HD3	2.43	0.54
1:C:1118:SER:O	1:C:1122:VAL:HG23	2.08	0.54
1:D:352:LYS:HE2	1:D:352:LYS:HA	1.89	0.54
1:D:715:MET:O	1:D:716:GLU:HB2	2.08	0.54
1:A:293:LEU:HD11	1:A:540:GLY:HA3	1.90	0.54
1:B:114:LYS:HB2	1:B:114:LYS:NZ	2.23	0.54
1:C:916:PRO:HD2	1:C:919:LYS:HB2	1.89	0.54
1:A:701:GLU:C	1:A:703:ASN:H	2.10	0.54
1:B:312:THR:CG2	1:B:338:TRP:HE1	2.20	0.54
1:C:516:TYR:HE2	1:C:533:MET:CE	2.20	0.54
1:D:299:LEU:CD2	1:D:309:LEU:HD11	2.37	0.54
1:D:317:LEU:HA	1:D:320:MET:CE	2.37	0.54
1:B:303:LYS:NZ	1:B:357:VAL:H	2.06	0.54
1:D:259:LEU:O	1:D:260:GLU:C	2.46	0.53
1:A:417:ILE:HD13	1:C:946:SER:HA	1.90	0.53
1:B:304:GLY:O	1:B:307:PRO:HD2	2.08	0.53
1:B:332:LEU:HA	1:B:335:PHE:HB3	1.90	0.53
1:B:945:ASN:HD21	1:B:951:LYS:HB3	1.73	0.53
1:C:593:MET:CE	1:C:604:ILE:HD12	2.39	0.53
1:D:149:TYR:OH	1:D:697:PHE:HB3	2.08	0.53
1:D:292:PHE:HE1	1:D:544:VAL:HG13	1.72	0.53
1:D:854:THR:HG22	1:D:855:LYS:HG2	1.90	0.53
1:C:140:MET:O	1:C:171:HIS:NE2	2.41	0.53
1:C:325:ASN:ND2	1:C:328:GLY:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:LYS:HD3	1:C:453:TYR:OH	2.07	0.53
1:A:1110:GLU:O	1:A:1111:SER:HB3	2.07	0.53
1:B:781:SER:O	1:B:784:ASP:N	2.41	0.53
1:C:540:GLY:HA2	1:C:557:TRP:CH2	2.44	0.53
1:D:6:PHE:CE1	1:D:10:ILE:CD1	2.91	0.53
1:A:516:TYR:CE2	1:A:533:MET:HE3	2.44	0.53
1:B:88:VAL:HG13	1:B:591:GLN:HG3	1.89	0.53
1:B:1223:LEU:HD21	1:B:1225:LEU:HD21	1.91	0.53
1:C:969:ARG:NH2	1:C:972:LEU:HD22	2.20	0.53
1:D:14:TRP:HB3	1:D:256:TYR:CG	2.44	0.53
1:D:55:LEU:HD22	1:D:59:GLU:HG2	1.91	0.53
1:B:36:MET:HE3	1:B:83:MET:CG	2.21	0.53
1:B:516:TYR:CE2	1:B:533:MET:CE	2.91	0.53
1:B:689:TYR:HB2	1:B:704:HIS:HD2	1.68	0.53
1:B:917:ILE:H	1:B:917:ILE:CD1	2.09	0.53
1:B:1193:ILE:O	1:B:1193:ILE:HG22	2.08	0.53
1:C:264:ILE:HG21	1:C:268:VAL:CG1	2.38	0.53
1:C:312:THR:CG2	1:C:338:TRP:HE1	2.21	0.53
1:A:169:SER:CB	1:A:676:ASP:OD1	2.57	0.53
1:C:152:HIS:HD2	1:C:704:HIS:NE2	2.07	0.53
1:C:593:MET:HG3	1:C:656:MET:SD	2.49	0.53
1:D:540:GLY:O	1:D:544:VAL:HG23	2.09	0.53
1:A:965:ILE:HD13	1:A:1122:VAL:HG13	1.89	0.53
1:C:312:THR:HG23	1:C:341:TYR:CB	2.39	0.53
1:C:359:TRP:HZ2	1:C:363:GLN:HE21	1.55	0.53
1:D:533:MET:HG3	1:D:561:TYR:CG	2.44	0.53
1:D:36:MET:SD	1:D:83:MET:HB3	2.48	0.52
1:C:339:LEU:HD21	1:C:570:VAL:HB	1.91	0.52
1:D:109:GLU:O	1:D:113:GLN:HB2	2.09	0.52
1:A:802:ARG:HD2	1:A:870:PRO:CB	2.39	0.52
1:A:864:ALA:HB3	1:A:895:LEU:CD1	2.39	0.52
1:C:963:PRO:HD3	1:C:1129:TYR:CZ	2.43	0.52
1:C:1111:SER:HB2	1:C:1191:THR:HA	1.90	0.52
1:D:6:PHE:CE1	1:D:10:ILE:HD12	2.45	0.52
1:C:606:VAL:O	1:C:608:TYR:N	2.43	0.52
1:D:704:HIS:CE1	1:D:706:ILE:H	2.28	0.52
1:B:98:ARG:HH11	1:B:644:ILE:HG12	1.73	0.52
1:B:140:MET:CE	1:B:143:LEU:HD13	2.40	0.52
1:C:140:MET:HE2	1:C:143:LEU:HD22	1.92	0.52
1:C:398:LEU:O	1:C:402:VAL:HB	2.10	0.52
1:A:592:LEU:HD22	1:A:596:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:GLU:O	1:A:658:PRO:HD2	2.10	0.52
1:A:883:SER:HA	1:A:911:GLU:HG2	1.91	0.52
1:B:626:GLU:O	1:B:627:VAL:CG2	2.57	0.52
1:B:933:TYR:CD1	1:B:1139:LYS:HE2	2.45	0.52
1:B:980:TYR:HD1	1:B:980:TYR:H	1.58	0.52
1:C:98:ARG:NH2	1:C:622:PHE:O	2.43	0.52
1:D:210:ILE:HA	1:D:223:LEU:HD11	1.92	0.52
1:D:310:LEU:CD2	1:D:314:LYS:HE3	2.40	0.52
1:A:137:THR:HG22	1:A:140:MET:H	1.74	0.52
1:A:1105:VAL:HG12	1:A:1105:VAL:O	2.10	0.52
1:B:796:SER:HB2	1:B:893:TYR:CE1	2.45	0.52
1:C:844:LYS:HG3	1:C:862:ILE:HB	1.92	0.52
1:D:676:ASP:CB	1:D:711:ILE:CG2	2.88	0.52
1:D:276:ARG:HH12	1:D:326:GLU:CA	2.10	0.52
1:D:820:LYS:HA	1:D:825:THR:HA	1.92	0.52
1:A:140:MET:O	1:A:171:HIS:NE2	2.33	0.52
1:A:325:ASN:ND2	1:A:328:GLY:H	2.07	0.52
1:B:458:ASP:OD1	1:B:461:SER:CB	2.58	0.51
1:B:592:LEU:O	1:B:596:LEU:HB2	2.09	0.51
1:C:516:TYR:HE2	1:C:533:MET:HE1	1.73	0.51
1:C:701:GLU:C	1:C:703:ASN:N	2.64	0.51
1:A:706:ILE:N	1:A:706:ILE:CD1	2.73	0.51
1:B:1138:GLN:O	1:B:1138:GLN:HG2	2.10	0.51
1:B:962:GLU:HG3	1:B:1169:ARG:HE	1.75	0.51
1:C:228:VAL:O	1:C:228:VAL:CG1	2.59	0.51
1:C:518:ASP:C	1:C:519:LYS:HD3	2.29	0.51
1:D:159:THR:HG23	1:D:1175:ASP:OD1	2.10	0.51
1:A:1111:SER:HA	1:A:1190:TYR:CD1	2.44	0.51
1:D:360:PHE:HA	1:D:363:GLN:HB3	1.92	0.51
1:A:1212:ASN:HD22	1:A:1215:GLY:H	1.56	0.51
1:B:201:CYS:HA	1:B:222:CYS:O	2.10	0.51
1:B:356:ASP:O	1:B:359:TRP:HB3	2.11	0.51
1:B:980:TYR:CD1	1:B:980:TYR:N	2.78	0.51
1:D:169:SER:OG	1:D:180:LYS:HD3	2.09	0.51
1:D:538:VAL:O	1:D:541:LEU:HB2	2.11	0.51
1:D:876:ARG:HG3	1:D:882:TYR:CE2	2.45	0.51
1:D:1111:SER:HB3	1:D:1191:THR:HA	1.92	0.51
1:A:301:LEU:O	1:A:303:LYS:N	2.42	0.51
1:C:264:ILE:O	1:C:264:ILE:HG22	2.11	0.51
1:C:417:ILE:O	1:C:419:PRO:HD3	2.11	0.51
1:D:589:PHE:HA	1:D:592:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:965:ILE:HD12	1:D:965:ILE:H	1.75	0.51
1:A:1191:THR:O	1:A:1191:THR:HG22	2.10	0.51
1:C:969:ARG:NH2	1:C:972:LEU:CD2	2.71	0.51
1:C:979:PHE:HD2	1:C:1039:UNK:CB	2.24	0.51
1:D:170:GLY:O	1:D:180:LYS:NZ	2.44	0.51
1:A:188:ILE:HG13	1:A:189:ARG:N	2.25	0.51
1:A:316:ALA:O	1:A:320:MET:HG3	2.11	0.51
1:A:1232:ASN:ND2	1:A:1235:ASP:H	2.09	0.51
1:B:102:PHE:HE1	1:B:599:ARG:NH1	2.09	0.51
1:D:91:ARG:HA	1:D:94:MET:HG3	1.91	0.51
1:B:876:ARG:NH1	1:B:920:GLU:OE2	2.43	0.51
1:C:219:HIS:CD2	1:C:254:ARG:NH1	2.72	0.51
1:C:355:ILE:H	1:C:355:ILE:HD12	1.75	0.51
1:D:32:LEU:HD13	1:D:75:ILE:HG13	1.92	0.51
1:B:1188:VAL:HG11	1:B:1202:LEU:HB2	1.93	0.51
1:C:254:ARG:NH2	1:C:275:GLU:OE1	2.44	0.51
1:C:969:ARG:HH21	1:C:972:LEU:HD23	1.76	0.51
1:D:534:THR:HG22	1:D:573:GLY:CA	2.40	0.51
1:B:798:TRP:O	1:B:800:PHE:N	2.44	0.50
1:C:195:ASN:ND2	1:C:197:ASN:H	2.09	0.50
1:C:622:PHE:O	1:C:623:TYR:CD2	2.64	0.50
1:D:155:ILE:HB	1:D:706:ILE:CG1	2.41	0.50
1:B:805:LYS:HB2	1:B:886:PHE:CE2	2.46	0.50
1:C:917:ILE:HD12	1:C:947:GLU:O	2.11	0.50
1:D:871:VAL:HG22	1:D:886:PHE:CE2	2.46	0.50
1:A:325:ASN:HD21	1:A:328:GLY:N	2.09	0.50
1:A:534:THR:CG2	1:A:573:GLY:HA2	2.41	0.50
1:A:864:ALA:CB	1:A:895:LEU:HD12	2.39	0.50
1:B:309:LEU:O	1:B:312:THR:HB	2.11	0.50
1:B:516:TYR:HE2	1:B:533:MET:HE2	1.77	0.50
1:C:169:SER:O	1:C:180:LYS:NZ	2.45	0.50
1:C:543:TRP:CD1	1:C:553:PRO:HG2	2.46	0.50
1:C:558:TYR:CE1	1:C:560:ARG:HG2	2.46	0.50
1:C:665:PRO:HA	1:C:668:LYS:HB2	1.92	0.50
1:D:85:ILE:HD13	1:D:143:LEU:HD21	1.93	0.50
1:D:1212:ASN:HD22	1:D:1215:GLY:H	1.58	0.50
1:A:969:ARG:NH1	1:A:972:LEU:CD2	2.74	0.50
1:B:312:THR:HG22	1:B:338:TRP:CD1	2.47	0.50
1:B:377:ARG:O	1:B:378:MET:C	2.50	0.50
1:D:1236:ARG:HB3	1:D:1239:VAL:HG22	1.94	0.50
1:A:768:VAL:CG1	1:A:858:LEU:HD13	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:948:THR:HG22	1:B:1146:ARG:NH2	2.26	0.50
1:C:798:TRP:O	1:C:801:LEU:HG	2.11	0.50
1:C:832:PRO:O	1:C:833:GLN:C	2.50	0.50
1:D:605:PRO:O	1:D:607:VAL:N	2.44	0.50
1:D:1111:SER:O	1:D:1112:ASP:HB3	2.11	0.50
1:A:1232:ASN:HD21	1:A:1235:ASP:H	1.60	0.50
1:C:554:SER:HB2	1:C:580:PHE:HB3	1.93	0.50
1:C:1171:MET:HB2	1:C:1233:LEU:HD11	1.94	0.50
1:A:770:HIS:CE1	1:A:858:LEU:HD22	2.46	0.50
1:B:589:PHE:HD1	1:B:592:LEU:HD12	1.76	0.50
1:B:677:LEU:HD13	1:B:708:ARG:HD2	1.94	0.50
1:D:310:LEU:HD21	1:D:314:LYS:HE3	1.93	0.50
1:D:542:GLN:HE21	1:D:542:GLN:HA	1.77	0.50
1:A:113:GLN:HE21	1:A:113:GLN:HA	1.76	0.50
1:B:1041:UNK:O	1:B:1042:UNK:C	2.60	0.50
1:C:248:LEU:HD23	1:C:248:LEU:C	2.33	0.50
1:C:666:ASP:OD1	1:C:666:ASP:N	2.32	0.50
1:D:212:LEU:HD21	1:D:548:TYR:CD1	2.46	0.50
1:D:441:GLY:HA2	1:D:462:ILE:HD13	1.93	0.50
1:A:1235:ASP:O	1:A:1237:GLN:HG3	2.12	0.50
1:C:221:PHE:HB3	1:C:250:LEU:HD12	1.94	0.50
1:A:152:HIS:HA	1:A:706:ILE:HG12	1.93	0.49
1:A:402:VAL:O	1:A:402:VAL:HG12	2.11	0.49
1:A:416:GLU:HB2	1:C:951:LYS:HZ1	1.77	0.49
1:A:417:ILE:O	1:A:419:PRO:HD3	2.12	0.49
1:A:947:GLU:HG3	1:A:947:GLU:O	2.10	0.49
1:C:862:ILE:HD12	1:C:862:ILE:N	2.26	0.49
1:D:770:HIS:CE1	1:D:858:LEU:HD22	2.47	0.49
1:C:965:ILE:HD12	1:C:965:ILE:H	1.76	0.49
1:D:159:THR:HA	1:D:162:GLN:CG	2.34	0.49
1:D:1173:ILE:HD11	1:D:1231:LEU:HB3	1.95	0.49
1:B:1203:PHE:O	1:B:1221:ARG:HD3	2.12	0.49
1:C:1210:GLY:HA2	1:C:1222:GLY:O	2.12	0.49
1:D:729:LYS:HZ1	1:D:904:ASN:HD21	1.59	0.49
1:A:144:THR:O	1:A:148:LYS:HG3	2.12	0.49
1:B:137:THR:HG22	1:B:138:GLU:N	2.27	0.49
1:B:512:LYS:NZ	1:B:569:ASP:OD1	2.45	0.49
1:C:518:ASP:O	1:C:519:LYS:HD3	2.12	0.49
1:C:928:VAL:HG21	1:C:1173:ILE:HG23	1.94	0.49
1:D:92:ALA:HA	1:D:558:TYR:HA	1.95	0.49
1:D:876:ARG:NH1	1:D:920:GLU:OE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:VAL:HG11	1:B:643:LYS:HB2	1.95	0.49
1:C:55:LEU:N	1:C:55:LEU:HD12	2.27	0.49
1:A:325:ASN:HD21	1:A:328:GLY:H	1.60	0.49
1:C:152:HIS:O	1:C:706:ILE:HD11	2.10	0.49
1:C:391:ILE:HD12	1:C:392:GLY:H	1.76	0.49
1:B:210:ILE:HA	1:B:223:LEU:CD1	2.43	0.49
1:C:36:MET:HE2	1:C:39:ILE:HD12	1.93	0.49
1:B:391:ILE:HD11	1:B:485:UNK:O	2.11	0.49
1:B:554:SER:HB2	1:B:580:PHE:HB3	1.94	0.49
1:B:954:VAL:HG21	1:B:1141:LEU:HD12	1.95	0.49
1:C:165:LYS:NZ	1:C:165:LYS:HB3	2.27	0.49
1:C:837:ARG:HD3	1:C:841:ARG:NH2	2.28	0.49
1:C:917:ILE:CD1	1:C:917:ILE:N	2.43	0.49
1:C:917:ILE:HG13	1:C:947:GLU:O	2.12	0.49
1:A:516:TYR:HE2	1:A:533:MET:HE3	1.78	0.49
1:B:1107:VAL:HG12	1:B:1108:SER:O	2.13	0.49
1:C:1232:ASN:HD22	1:C:1234:SER:H	1.60	0.49
1:D:219:HIS:HD2	1:D:254:ARG:NH1	2.10	0.49
1:A:797:ARG:O	1:A:798:TRP:O	2.30	0.49
1:B:622:PHE:HD2	1:B:622:PHE:C	2.16	0.49
1:C:365:GLU:O	1:C:369:LEU:HG	2.13	0.49
1:D:804:SER:HB2	1:D:868:VAL:HB	1.95	0.49
1:D:876:ARG:HG3	1:D:882:TYR:CZ	2.48	0.49
1:D:945:ASN:ND2	1:D:1143:LYS:N	2.60	0.49
1:A:146:ASN:O	1:A:149:TYR:HB3	2.12	0.48
1:B:933:TYR:CE2	1:B:1139:LYS:HB2	2.48	0.48
1:C:530:LEU:C	1:C:532:GLU:H	2.16	0.48
1:C:605:PRO:O	1:C:606:VAL:C	2.51	0.48
1:D:93:LYS:HB3	1:D:97:GLN:NE2	2.28	0.48
1:D:747:THR:CG2	1:D:770:HIS:HB2	2.43	0.48
1:D:852:GLN:HG2	1:D:857:ILE:O	2.13	0.48
1:A:302:LYS:O	1:A:303:LYS:HE2	2.13	0.48
1:A:1122:VAL:HG12	1:A:1202:LEU:HD13	1.94	0.48
1:B:33:TYR:OH	1:B:200:HIS:HD2	1.95	0.48
1:B:534:THR:CG2	1:B:573:GLY:N	2.76	0.48
1:B:744:LEU:HD22	1:B:798:TRP:CD1	2.48	0.48
1:B:965:ILE:H	1:B:965:ILE:HG13	1.44	0.48
1:C:391:ILE:HD12	1:C:392:GLY:N	2.28	0.48
1:D:507:ARG:O	1:D:511:TRP:N	2.36	0.48
1:D:965:ILE:HD12	1:D:965:ILE:N	2.28	0.48
1:B:682:ASN:O	1:B:705:CYS:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:ARG:HH12	1:A:972:LEU:HD23	1.79	0.48
1:B:1223:LEU:CD2	1:B:1225:LEU:HD21	2.43	0.48
1:C:416:GLU:HG2	1:C:417:ILE:H	1.77	0.48
1:C:516:TYR:CE2	1:C:533:MET:CE	2.94	0.48
1:D:933:TYR:CD1	1:D:1139:LYS:HE2	2.49	0.48
1:D:964:ASN:H	1:D:965:ILE:HD12	1.79	0.48
1:A:963:PRO:HD3	1:A:1129:TYR:CE1	2.49	0.48
1:B:152:HIS:HD2	1:B:706:ILE:HB	1.69	0.48
1:D:342:LEU:HB3	1:D:567:ILE:CG2	2.43	0.48
1:D:542:GLN:HE21	1:D:542:GLN:CA	2.26	0.48
1:A:313:PHE:CZ	1:A:317:LEU:HD22	2.49	0.48
1:A:1050:UNK:O	1:A:1091:LYS:N	2.46	0.48
1:B:1137:GLU:HG2	1:B:1138:GLN:N	2.26	0.48
1:C:593:MET:HE2	1:C:604:ILE:HD12	1.96	0.48
1:A:156:THR:N	1:A:706:ILE:HD11	2.28	0.48
1:A:426:VAL:HG13	1:A:433:LEU:HD13	1.94	0.48
1:A:535:GLU:HG2	1:A:576:GLN:OE1	2.14	0.48
1:B:131:ASN:N	1:B:131:ASN:OD1	2.45	0.48
1:B:543:TRP:CD1	1:B:553:PRO:HG2	2.49	0.48
1:B:927:VAL:HG21	1:B:1149:ILE:HG13	1.93	0.48
1:D:565:PRO:O	1:D:566:ARG:HG2	2.12	0.48
1:A:816:TYR:CD1	1:A:816:TYR:N	2.80	0.48
1:D:61:TYR:OH	1:D:143:LEU:HD12	2.14	0.48
1:D:292:PHE:CE1	1:D:544:VAL:HG13	2.49	0.48
1:D:390:LEU:O	1:D:394:VAL:HG23	2.13	0.48
1:A:1099:GLU:OE2	1:A:1102:LYS:HE3	2.14	0.48
1:B:916:PRO:HD2	1:B:919:LYS:HB2	1.95	0.48
1:B:1112:ASP:OD1	1:B:1112:ASP:N	2.46	0.48
1:C:354:ASP:N	1:C:354:ASP:OD1	2.45	0.48
1:A:708:ARG:HH11	1:A:708:ARG:HB2	1.79	0.48
1:A:793:ILE:HD13	1:A:793:ILE:HA	1.75	0.48
1:A:1172:TYR:CD1	1:A:1179:VAL:HB	2.48	0.48
1:B:169:SER:OG	1:B:180:LYS:HD2	2.14	0.48
1:B:417:ILE:HG13	1:B:454:TYR:HD1	1.78	0.48
1:B:622:PHE:C	1:B:622:PHE:CD2	2.87	0.48
1:C:363:GLN:O	1:C:367:ILE:HD13	2.14	0.48
1:C:587:LYS:N	1:C:590:GLN:HE21	2.02	0.48
1:C:744:LEU:HD21	1:C:897:LEU:HA	1.96	0.48
1:C:873:GLY:HA2	1:C:909:TYR:CE2	2.48	0.48
1:A:336:SER:HA	1:A:339:LEU:HB2	1.94	0.47
1:A:741:LEU:HD22	1:A:769:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:PRO:HD2	1:A:897:LEU:HD12	1.96	0.47
1:B:576:GLN:HG3	1:B:577:ASN:N	2.28	0.47
1:B:918:ASN:ND2	1:B:918:ASN:H	2.10	0.47
1:C:527:THR:HB	1:C:528:ASP:H	1.44	0.47
1:D:284:VAL:HG21	1:D:313:PHE:CG	2.48	0.47
1:B:1165:HIS:O	1:B:1168:ASP:HB2	2.13	0.47
1:A:94:MET:O	1:A:98:ARG:HB3	2.14	0.47
1:B:559:TYR:OH	1:B:565:PRO:HD3	2.14	0.47
1:B:571:ILE:C	1:B:573:GLY:H	2.18	0.47
1:C:16:GLN:HE22	1:C:799:PRO:HG3	1.79	0.47
1:D:142:LYS:O	1:D:146:ASN:ND2	2.46	0.47
1:D:1113:SER:HA	1:D:1189:GLY:HA2	1.96	0.47
1:A:798:TRP:HE3	1:A:799:PRO:HD3	1.78	0.47
1:A:1212:ASN:OD1	1:A:1212:ASN:N	2.42	0.47
1:B:528:ASP:HA	1:B:531:LYS:HB2	1.96	0.47
1:B:537:TYR:O	1:B:540:GLY:N	2.47	0.47
1:D:373:ARG:O	1:D:376:THR:OG1	2.20	0.47
1:A:387:GLN:O	1:A:391:ILE:HG13	2.14	0.47
1:B:10:ILE:HG12	1:B:14:TRP:HZ3	1.77	0.47
1:B:676:ASP:CB	1:B:711:ILE:HG22	2.44	0.47
1:D:189:ARG:NH2	1:D:723:GLY:O	2.38	0.47
1:D:917:ILE:CD1	1:D:947:GLU:O	2.63	0.47
1:A:40:LEU:HD22	1:A:143:LEU:HD11	1.96	0.47
1:A:144:THR:HG22	1:A:148:LYS:HE3	1.97	0.47
1:A:430:LEU:O	1:A:434:LYS:HG3	2.15	0.47
1:A:471:UNK:C	1:A:473:UNK:N	2.77	0.47
1:A:592:LEU:CD2	1:A:596:LEU:HD12	2.45	0.47
1:A:701:GLU:C	1:A:703:ASN:N	2.68	0.47
1:C:152:HIS:CD2	1:C:704:HIS:NE2	2.83	0.47
1:C:696:LEU:CD2	1:C:1206:GLU:HB3	2.45	0.47
1:C:1087:ASP:O	1:C:1088:SER:C	2.52	0.47
1:D:220:HIS:CE1	1:D:735:LEU:HB2	2.50	0.47
1:B:544:VAL:O	1:B:547:TYR:HB3	2.15	0.47
1:C:113:GLN:O	1:C:114:LYS:C	2.53	0.47
1:C:806:LEU:HA	1:C:868:VAL:HG12	1.96	0.47
1:C:809:LEU:C	1:C:810:ILE:HG12	2.34	0.47
1:A:606:VAL:C	1:A:607:VAL:HG23	2.34	0.47
1:C:965:ILE:HD12	1:C:965:ILE:N	2.29	0.47
1:C:1086:ALA:O	1:C:1087:ASP:C	2.52	0.47
1:D:217:HIS:CE1	1:D:275:GLU:HB3	2.50	0.47
1:A:959:LEU:HD21	1:A:1137:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ILE:HD12	1:B:367:ILE:H	1.80	0.47
1:B:387:GLN:HG2	1:B:432:PHE:CZ	2.49	0.47
1:B:828:ILE:O	1:B:828:ILE:HG22	2.15	0.47
1:C:1042:UNK:O	1:C:1045:UNK:N	2.48	0.47
1:D:222:CYS:SG	1:D:249:HIS:CE1	3.08	0.47
1:D:689:TYR:HB2	1:D:704:HIS:CD2	2.50	0.47
1:A:1116:LYS:HG3	1:A:1216:ARG:HG3	1.97	0.46
1:A:1195:LYS:HG2	1:A:1196:ASN:HD22	1.80	0.46
1:B:98:ARG:NH1	1:B:644:ILE:HG12	2.30	0.46
1:B:219:HIS:CE1	1:B:251:SER:HB2	2.50	0.46
1:B:830:ARG:CG	1:B:831:LYS:N	2.78	0.46
1:C:165:LYS:HB2	1:C:165:LYS:HZ2	1.80	0.46
1:C:918:ASN:HA	1:C:944:TYR:CZ	2.50	0.46
1:D:334:ARG:HG3	1:D:334:ARG:HH11	1.81	0.46
1:A:622:PHE:HZ	1:A:648:ASP:HB3	1.80	0.46
1:A:826:LYS:CG	1:A:827:VAL:N	2.66	0.46
1:A:952:LEU:CD1	1:A:1149:ILE:HD11	2.44	0.46
1:A:1232:ASN:ND2	1:A:1234:SER:H	2.13	0.46
1:B:335:PHE:O	1:B:335:PHE:HD1	1.97	0.46
1:A:540:GLY:HA2	1:A:557:TRP:CZ2	2.50	0.46
1:B:1163:ARG:HG3	1:B:1237:GLN:OE1	2.15	0.46
1:C:534:THR:CG2	1:C:573:GLY:HA3	2.41	0.46
1:D:395:LYS:O	1:D:396:PRO:C	2.54	0.46
1:D:589:PHE:CD1	1:D:589:PHE:N	2.84	0.46
1:D:1116:LYS:HG3	1:D:1216:ARG:CD	2.45	0.46
1:A:189:ARG:HA	1:A:194:TYR:CG	2.50	0.46
1:A:417:ILE:HG12	1:A:454:TYR:CD1	2.50	0.46
1:A:712:PRO:O	1:A:713:GLU:HB3	2.16	0.46
1:B:588:PRO:O	1:B:591:GLN:HB3	2.15	0.46
1:D:26:ILE:HB	1:D:27:PRO:HD2	1.98	0.46
1:D:1207:ILE:O	1:D:1208:ILE:C	2.54	0.46
1:A:534:THR:HG22	1:A:535:GLU:N	2.30	0.46
1:A:1181:LEU:HG	1:A:1182:HIS:CD2	2.50	0.46
1:B:43:CYS:HB2	1:B:64:ILE:HD13	1.98	0.46
1:C:128:PHE:CE2	1:C:130:SER:HA	2.50	0.46
1:C:154:LYS:HD2	1:C:154:LYS:HA	1.56	0.46
1:C:952:LEU:HD11	1:C:1144:VAL:HG21	1.98	0.46
1:A:91:ARG:C	1:A:93:LYS:N	2.69	0.46
1:A:195:ASN:HD22	1:A:196:PRO:HD2	1.79	0.46
1:A:260:GLU:O	1:A:314:LYS:HE2	2.15	0.46
1:A:303:LYS:HG2	1:A:355:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ILE:HD11	1:B:166:VAL:CG2	2.37	0.46
1:B:209:LEU:HB3	1:B:223:LEU:CD2	2.46	0.46
1:D:76:LYS:HD3	1:D:160:ARG:CZ	2.45	0.46
1:D:357:VAL:HG12	1:D:361:ASN:ND2	2.30	0.46
1:A:798:TRP:O	1:A:800:PHE:N	2.49	0.46
1:A:821:SER:HB3	1:A:824:LEU:O	2.16	0.46
1:C:850:ASN:ND2	1:C:853:ARG:HH12	2.13	0.46
1:D:155:ILE:CG2	1:D:706:ILE:HD12	2.46	0.46
1:D:1116:LYS:HG3	1:D:1216:ARG:HD2	1.98	0.46
1:A:96:GLN:H	1:A:96:GLN:NE2	2.03	0.46
1:B:1171:MET:HB3	1:B:1173:ILE:HD11	1.97	0.46
1:D:58:GLU:HG2	1:D:59:GLU:N	2.30	0.46
1:D:210:ILE:HA	1:D:223:LEU:HD13	1.97	0.46
1:D:516:TYR:OH	1:D:569:ASP:OD2	2.19	0.46
1:D:706:ILE:N	1:D:706:ILE:CD1	2.74	0.46
1:D:927:VAL:HG21	1:D:1149:ILE:HG12	1.97	0.46
1:A:663:LEU:HB3	1:A:667:GLU:HB2	1.97	0.46
1:A:708:ARG:HH11	1:A:708:ARG:CB	2.28	0.46
1:A:798:TRP:CG	1:A:799:PRO:HD3	2.51	0.46
1:B:264:ILE:HG23	1:B:267:SER:HB2	1.98	0.46
1:B:704:HIS:CE1	1:B:706:ILE:H	2.33	0.46
1:B:798:TRP:HB3	1:B:799:PRO:HD3	1.98	0.46
1:D:325:ASN:HD21	1:D:328:GLY:HA2	1.80	0.46
1:D:798:TRP:O	1:D:799:PRO:C	2.53	0.46
1:D:1204:ASP:O	1:D:1221:ARG:NH1	2.49	0.46
1:A:405:LYS:HE3	1:A:405:LYS:HB2	1.65	0.46
1:B:704:HIS:HE1	1:B:706:ILE:O	1.99	0.46
1:B:1181:LEU:O	1:B:1182:HIS:CB	2.60	0.46
1:B:1191:THR:HG23	1:B:1193:ILE:HD13	1.97	0.46
1:C:31:ASN:HB3	1:C:33:TYR:CZ	2.51	0.46
1:C:212:LEU:HD21	1:C:548:TYR:HD1	1.75	0.46
1:D:309:LEU:O	1:D:312:THR:HB	2.16	0.46
1:D:952:LEU:HD21	1:D:1149:ILE:HD13	1.96	0.46
1:A:177:GLY:O	1:A:181:ILE:HG13	2.15	0.45
1:B:296:LEU:CB	1:B:297:PRO:CD	2.79	0.45
1:C:1102:LYS:HB2	1:C:1103:PRO:CD	2.38	0.45
1:A:744:LEU:HD22	1:A:798:TRP:CE2	2.42	0.45
1:A:969:ARG:HH11	1:A:972:LEU:HD22	1.81	0.45
1:B:284:VAL:HG21	1:B:313:PHE:CG	2.50	0.45
1:B:296:LEU:HD13	1:B:567:ILE:HG12	1.97	0.45
1:B:486:UNK:O	1:B:487:UNK:C	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:LEU:O	1:C:848:LYS:C	2.54	0.45
1:C:1087:ASP:O	1:C:1090:LEU:N	2.49	0.45
1:C:1173:ILE:HG13	1:C:1231:LEU:HB2	1.96	0.45
1:A:29:PHE:CD2	1:A:75:ILE:HG23	2.52	0.45
1:A:303:LYS:HG2	1:A:355:ILE:HD12	1.98	0.45
1:A:811:THR:CG2	1:A:812:GLU:N	2.79	0.45
1:A:946:SER:OG	1:A:947:GLU:N	2.49	0.45
1:A:1041:UNK:O	1:A:1042:UNK:C	2.65	0.45
1:B:531:LYS:HB3	1:B:531:LYS:HZ2	1.77	0.45
1:B:812:GLU:OE2	1:B:841:ARG:NH2	2.49	0.45
1:C:85:ILE:HD13	1:C:143:LEU:HD21	1.98	0.45
1:C:156:THR:OG1	1:C:705:CYS:N	2.46	0.45
1:C:264:ILE:CG2	1:C:264:ILE:O	2.64	0.45
1:C:875:VAL:HG12	1:C:885:SER:HB2	1.97	0.45
1:D:280:ASP:OD1	1:D:323:TYR:HB3	2.16	0.45
1:A:817:GLU:O	1:A:827:VAL:HA	2.17	0.45
1:A:971:LYS:HE3	1:A:975:GLN:OE1	2.16	0.45
1:B:297:PRO:HG2	1:B:298:ASP:H	1.81	0.45
1:C:858:LEU:HD12	1:C:858:LEU:HA	1.78	0.45
1:A:795:TYR:HA	1:A:802:ARG:O	2.16	0.45
1:C:968:VAL:O	1:C:971:LYS:HB3	2.16	0.45
1:A:284:VAL:HG13	1:A:338:TRP:CZ2	2.52	0.45
1:A:417:ILE:HD13	1:C:945:ASN:O	2.16	0.45
1:A:419:PRO:HA	1:A:454:TYR:HB3	1.97	0.45
1:B:22:ASP:OD2	1:B:22:ASP:C	2.55	0.45
1:B:296:LEU:HB2	1:B:299:LEU:HD11	1.98	0.45
1:C:33:TYR:OH	1:C:200:HIS:CD2	2.61	0.45
1:C:510:GLU:O	1:C:514:GLN:HB2	2.15	0.45
1:D:313:PHE:HE1	1:D:317:LEU:HD13	1.80	0.45
1:D:589:PHE:CE2	1:D:605:PRO:HG3	2.51	0.45
1:D:929:PHE:HD1	1:D:1149:ILE:HD12	1.80	0.45
1:D:967:LYS:O	1:D:970:ALA:HB3	2.16	0.45
1:A:624:PRO:HB2	1:A:626:GLU:O	2.17	0.45
1:A:744:LEU:HB2	1:A:798:TRP:NE1	2.32	0.45
1:A:800:PHE:O	1:A:801:LEU:C	2.55	0.45
1:A:1039:UNK:O	1:A:1040:UNK:C	2.65	0.45
1:A:1112:ASP:CG	1:A:1113:SER:H	2.21	0.45
1:B:264:ILE:HG22	1:B:265:THR:H	1.77	0.45
1:B:731:GLY:C	1:B:733:SER:H	2.21	0.45
1:B:744:LEU:HD13	1:B:899:VAL:HG22	1.99	0.45
1:C:209:LEU:HB3	1:C:223:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:PHE:HB3	1:C:250:LEU:HB2	1.98	0.45
1:D:331:ASN:OD1	1:D:334:ARG:HG2	2.16	0.45
1:D:589:PHE:N	1:D:589:PHE:HD1	2.14	0.45
1:A:571:ILE:O	1:A:574:ILE:HG12	2.17	0.45
1:A:918:ASN:HD22	1:A:918:ASN:N	2.14	0.45
1:A:1092:THR:O	1:A:1093:VAL:CG2	2.52	0.45
1:A:1093:VAL:HG12	1:A:1097:LEU:HD12	1.98	0.45
1:B:816:TYR:CD1	1:B:816:TYR:N	2.85	0.45
1:C:112:LEU:O	1:C:113:GLN:HB2	2.17	0.45
1:C:195:ASN:HD22	1:C:196:PRO:HD2	1.81	0.45
1:C:393:ALA:O	1:C:396:PRO:HD2	2.16	0.45
1:D:754:SER:HA	1:D:762:SER:O	2.17	0.45
1:A:325:ASN:HD21	1:A:328:GLY:HA2	1.80	0.45
1:A:712:PRO:O	1:A:713:GLU:HB2	2.16	0.45
1:A:798:TRP:O	1:A:801:LEU:N	2.49	0.45
1:A:933:TYR:OH	1:A:1137:GLU:HG2	2.16	0.45
1:B:965:ILE:O	1:B:966:GLY:C	2.56	0.45
1:D:54:ARG:HG2	1:D:55:LEU:N	2.31	0.45
1:D:140:MET:HB3	1:D:171:HIS:NE2	2.31	0.45
1:D:155:ILE:HB	1:D:706:ILE:CD1	2.47	0.45
1:A:98:ARG:HB2	1:A:595:VAL:HA	1.99	0.44
1:A:606:VAL:O	1:A:607:VAL:CG2	2.61	0.44
1:B:85:ILE:HD13	1:B:143:LEU:HD21	1.99	0.44
1:B:250:LEU:HD23	1:B:253:LEU:HD23	1.99	0.44
1:B:477:UNK:O	1:B:481:UNK:N	2.50	0.44
1:B:1111:SER:HB2	1:B:1190:TYR:O	2.17	0.44
1:C:696:LEU:HD21	1:C:1206:GLU:HB3	1.97	0.44
1:C:820:LYS:HG2	1:C:822:GLY:H	1.82	0.44
1:D:87:GLY:C	1:D:135:PRO:HG3	2.38	0.44
1:D:299:LEU:HD22	1:D:309:LEU:HD13	1.99	0.44
1:D:592:LEU:O	1:D:595:VAL:O	2.35	0.44
1:D:945:ASN:HD22	1:D:1143:LYS:HA	1.82	0.44
1:A:72:PHE:C	1:A:72:PHE:CD2	2.91	0.44
1:A:134:THR:O	1:A:140:MET:HG3	2.17	0.44
1:A:155:ILE:CG2	1:A:706:ILE:HG13	2.47	0.44
1:A:417:ILE:HG12	1:A:454:TYR:CE1	2.52	0.44
1:A:446:HIS:CD2	1:A:450:LYS:HD2	2.52	0.44
1:A:219:HIS:HA	1:A:254:ARG:HH11	1.83	0.44
1:B:700:ILE:O	1:B:701:GLU:O	2.36	0.44
1:B:1119:MET:SD	1:B:1216:ARG:HD2	2.58	0.44
1:D:178:GLN:NE2	1:D:206:ASP:OD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:O	1:A:345:PHE:HB3	2.17	0.44
1:A:1166:LEU:CD2	1:A:1189:GLY:HA2	2.48	0.44
1:B:388:LYS:O	1:B:389:LYS:C	2.53	0.44
1:B:798:TRP:CG	1:B:799:PRO:N	2.81	0.44
1:B:931:GLY:HA2	1:B:1240:TYR:HA	1.98	0.44
1:B:1149:ILE:HD12	1:B:1149:ILE:HA	1.52	0.44
1:C:58:GLU:O	1:C:62:SER:HB2	2.17	0.44
1:C:182:MET:HE2	1:C:185:ILE:HD12	1.99	0.44
1:C:597:PRO:C	1:C:599:ARG:H	2.21	0.44
1:C:1102:LYS:O	1:C:1104:PHE:N	2.51	0.44
1:D:14:TRP:O	1:D:17:ILE:HG23	2.18	0.44
1:D:928:VAL:CG2	1:D:1173:ILE:HG22	2.48	0.44
1:D:1139:LYS:HE3	1:D:1141:LEU:HD21	2.00	0.44
1:A:676:ASP:HB2	1:A:711:ILE:CG2	2.48	0.44
1:A:719:LYS:HZ1	1:C:716:GLU:HB3	1.83	0.44
1:A:969:ARG:HH11	1:A:972:LEU:CD2	2.31	0.44
1:B:689:TYR:CB	1:B:704:HIS:HD2	2.29	0.44
1:B:689:TYR:CD2	1:B:690:LYS:N	2.86	0.44
1:B:704:HIS:ND1	1:B:704:HIS:C	2.71	0.44
1:B:774:LEU:O	1:B:775:TYR:CD2	2.71	0.44
1:B:945:ASN:ND2	1:B:951:LYS:HB3	2.33	0.44
1:C:36:MET:O	1:C:39:ILE:N	2.50	0.44
1:C:706:ILE:CG2	1:C:707:GLU:N	2.80	0.44
1:C:707:GLU:OE1	1:C:707:GLU:O	2.36	0.44
1:C:845:MET:O	1:C:849:SER:HB2	2.17	0.44
1:A:259:LEU:CB	1:A:767:MET:HE2	2.46	0.44
1:B:154:LYS:O	1:B:155:ILE:C	2.55	0.44
1:B:543:TRP:NE1	1:B:553:PRO:HD2	2.33	0.44
1:B:704:HIS:C	1:B:704:HIS:HD1	2.21	0.44
1:C:154:LYS:HG3	1:C:161:TRP:CE2	2.53	0.44
1:C:206:ASP:OD1	1:C:208:ASP:HB2	2.17	0.44
1:C:259:LEU:HD11	1:C:741:LEU:CD1	2.47	0.44
1:C:516:TYR:CE2	1:C:530:LEU:HD12	2.52	0.44
1:C:534:THR:HG21	1:C:572:LYS:C	2.38	0.44
1:D:268:VAL:C	1:D:270:PHE:H	2.21	0.44
1:A:459:LEU:O	1:A:462:ILE:HD12	2.18	0.44
1:B:471:UNK:C	1:B:473:UNK:N	2.79	0.44
1:B:531:LYS:HG2	1:B:572:LYS:HB3	1.99	0.44
1:C:55:LEU:HD12	1:C:55:LEU:H	1.83	0.44
1:C:162:GLN:HG2	1:C:681:PHE:CD1	2.52	0.44
1:D:787:LYS:HA	1:D:827:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:HB	1:A:265:THR:H	1.52	0.44
1:B:6:PHE:O	1:B:10:ILE:HB	2.18	0.44
1:B:250:LEU:CD2	1:B:253:LEU:HD23	2.47	0.44
1:B:391:ILE:H	1:B:391:ILE:HG13	1.60	0.44
1:B:712:PRO:O	1:B:713:GLU:CB	2.64	0.44
1:B:971:LYS:HG2	1:B:975:GLN:HE21	1.83	0.44
1:C:362:GLN:O	1:C:365:GLU:HB3	2.18	0.44
1:C:959:LEU:HD21	1:C:1137:GLU:OE2	2.18	0.44
1:D:387:GLN:O	1:D:391:ILE:HG12	2.17	0.44
1:B:286:PHE:CZ	1:B:548:TYR:CD2	3.05	0.44
1:B:933:TYR:CZ	1:B:1139:LYS:HB2	2.53	0.44
1:C:293:LEU:HD21	1:C:540:GLY:HA3	2.00	0.44
1:C:530:LEU:O	1:C:534:THR:HB	2.18	0.44
1:D:56:SER:HB3	1:D:59:GLU:HB2	1.98	0.44
1:D:340:LYS:HA	1:D:340:LYS:NZ	2.31	0.44
1:D:507:ARG:HA	1:D:510:GLU:HB3	2.00	0.44
1:D:768:VAL:HG13	1:D:858:LEU:HD13	2.00	0.44
1:A:109:GLU:O	1:A:113:GLN:HB3	2.18	0.43
1:A:1111:SER:HB2	1:A:1191:THR:HA	1.99	0.43
1:C:352:LYS:HD2	1:C:354:ASP:O	2.18	0.43
1:A:259:LEU:HB3	1:A:767:MET:HE2	1.91	0.43
1:B:682:ASN:HA	1:B:683:PRO:HD2	1.49	0.43
1:C:307:PRO:HG2	1:C:764:GLN:CG	2.48	0.43
1:C:597:PRO:HD2	1:C:600:SER:HB2	2.00	0.43
1:C:876:ARG:NH1	1:C:920:GLU:OE1	2.51	0.43
1:D:1114:LEU:HD12	1:D:1188:VAL:HG12	2.00	0.43
1:A:516:TYR:CE2	1:A:533:MET:CE	3.01	0.43
1:A:843:LEU:HD12	1:A:843:LEU:HA	1.74	0.43
1:B:14:TRP:HB3	1:B:256:TYR:CG	2.53	0.43
1:B:534:THR:HG22	1:B:573:GLY:N	2.32	0.43
1:B:807:LEU:O	1:B:808:SER:HB3	2.18	0.43
1:C:561:TYR:N	1:C:561:TYR:CD2	2.85	0.43
1:C:1123:GLU:O	1:C:1127:ILE:HG13	2.18	0.43
1:D:312:THR:CG2	1:D:338:TRP:HE1	2.03	0.43
1:A:220:HIS:CE1	1:A:735:LEU:HB2	2.53	0.43
1:A:262:GLU:C	1:A:264:ILE:N	2.72	0.43
1:A:744:LEU:HA	1:A:744:LEU:HD12	1.62	0.43
1:A:826:LYS:CD	1:A:827:VAL:H	2.31	0.43
1:B:1191:THR:HG22	1:B:1191:THR:O	2.18	0.43
1:C:426:VAL:HG12	1:C:427:ARG:N	2.33	0.43
1:D:32:LEU:HA	1:D:201:CYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:LYS:HA	1:D:542:GLN:OE1	2.18	0.43
1:D:679:PHE:N	1:D:679:PHE:HD1	2.16	0.43
1:A:11:SER:O	1:A:15:PRO:HA	2.18	0.43
1:B:182:MET:HE3	1:B:185:ILE:HD12	2.00	0.43
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.79	0.43
1:B:1212:ASN:O	1:B:1213:PHE:C	2.56	0.43
1:C:152:HIS:CD2	1:C:706:ILE:HB	2.54	0.43
1:C:273:ASP:O	1:C:277:VAL:HG23	2.18	0.43
1:C:1232:ASN:HD22	1:C:1232:ASN:C	2.19	0.43
1:A:311:GLN:HG2	1:A:364:LEU:HD12	2.00	0.43
1:A:1111:SER:HA	1:A:1190:TYR:CE1	2.53	0.43
1:B:346:GLU:OE1	1:B:566:ARG:HB3	2.18	0.43
1:B:527:THR:HB	1:B:528:ASP:H	1.57	0.43
1:B:592:LEU:O	1:B:596:LEU:HD12	2.19	0.43
1:C:101:ARG:HG3	1:C:131:ASN:CG	2.39	0.43
1:C:870:PRO:HD2	1:C:887:ASN:CB	2.49	0.43
1:D:103:ARG:O	1:D:106:MET:HB3	2.19	0.43
1:D:266:ASP:O	1:D:267:SER:CB	2.61	0.43
1:D:832:PRO:HA	1:D:836:GLU:OE1	2.18	0.43
1:A:133:ILE:HG23	1:A:140:MET:HE1	2.00	0.43
1:A:589:PHE:HA	1:A:592:LEU:HB2	1.99	0.43
1:A:820:LYS:HG3	1:A:820:LYS:O	2.18	0.43
1:A:1112:ASP:CG	1:A:1113:SER:N	2.72	0.43
1:B:220:HIS:HE1	1:B:735:LEU:N	2.00	0.43
1:B:566:ARG:HB3	1:B:566:ARG:HE	1.72	0.43
1:B:684:GLN:HE21	1:B:684:GLN:HB2	1.59	0.43
1:C:156:THR:H	1:C:706:ILE:HD11	1.83	0.43
1:C:950:LEU:HD23	1:C:1144:VAL:O	2.18	0.43
1:D:303:LYS:CE	1:D:356:ASP:HA	2.36	0.43
1:D:343:SER:HA	1:D:568:SER:OG	2.18	0.43
1:B:516:TYR:HE2	1:B:533:MET:CE	2.31	0.43
1:D:61:TYR:O	1:D:65:PHE:CD2	2.72	0.43
1:D:664:SER:HB3	1:D:665:PRO:HD2	2.00	0.43
1:A:101:ARG:HD3	1:A:595:VAL:HG13	2.01	0.43
1:A:140:MET:HB3	1:A:171:HIS:NE2	2.33	0.43
1:B:7:PHE:O	1:B:8:HIS:C	2.57	0.43
1:B:303:LYS:HA	1:B:303:LYS:HD2	1.83	0.43
1:B:872:ASN:ND2	1:B:887:ASN:HD22	2.10	0.43
1:C:319:HIS:HE1	1:C:375:ARG:HG3	1.84	0.43
1:C:593:MET:CB	1:C:652:LEU:HD11	2.49	0.43
1:C:1085:GLU:O	1:C:1086:ALA:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:932:ASP:O	1:D:933:TYR:C	2.57	0.43
1:D:1175:ASP:OD1	1:D:1175:ASP:C	2.56	0.43
1:A:14:TRP:O	1:A:17:ILE:HG23	2.19	0.43
1:A:526:ASP:C	1:A:527:THR:OG1	2.57	0.43
1:A:622:PHE:O	1:A:623:TYR:CG	2.72	0.43
1:B:159:THR:O	1:B:162:GLN:HG2	2.19	0.43
1:B:798:TRP:HA	1:B:801:LEU:HD23	2.01	0.43
1:C:355:ILE:HG22	1:C:359:TRP:CD1	2.53	0.43
1:C:730:LEU:O	1:C:731:GLY:C	2.57	0.43
1:D:604:ILE:O	1:D:606:VAL:N	2.52	0.43
1:D:713:GLU:HG3	1:D:714:SER:N	2.33	0.43
1:A:217:HIS:CG	1:A:723:GLY:HA2	2.53	0.42
1:A:461:SER:O	1:A:461:SER:OG	2.32	0.42
1:A:542:GLN:NE2	1:A:542:GLN:HA	2.34	0.42
1:B:312:THR:CG2	1:B:338:TRP:NE1	2.80	0.42
1:B:901:ASP:CG	1:B:902:VAL:H	2.22	0.42
1:C:212:LEU:HD11	1:C:548:TYR:CE1	2.54	0.42
1:C:677:LEU:HD22	1:C:708:ARG:HH12	1.84	0.42
1:C:816:TYR:CD1	1:C:816:TYR:N	2.87	0.42
1:C:834:ASP:HA	1:C:837:ARG:HB3	2.01	0.42
1:C:949:ARG:HH21	1:C:1145:PRO:HB3	1.83	0.42
1:D:195:ASN:HD22	1:D:196:PRO:CD	2.26	0.42
1:B:417:ILE:CG1	1:B:454:TYR:CD1	2.99	0.42
1:C:133:ILE:HA	1:C:140:MET:SD	2.59	0.42
1:C:351:GLU:OE2	1:C:507:ARG:NH1	2.51	0.42
1:C:622:PHE:C	1:C:623:TYR:CG	2.93	0.42
1:A:171:HIS:CE1	1:A:172:GLU:OE2	2.72	0.42
1:A:597:PRO:C	1:A:599:ARG:H	2.23	0.42
1:A:1227:SER:O	1:A:1229:PHE:N	2.52	0.42
1:B:1040:UNK:O	1:B:1041:UNK:C	2.67	0.42
1:C:67:TYR:O	1:C:70:HIS:N	2.52	0.42
1:C:258:ALA:HA	1:C:274:PHE:CE1	2.54	0.42
1:D:1207:ILE:HG22	1:D:1209:ALA:H	1.83	0.42
1:A:689:TYR:HB3	1:A:700:ILE:HB	2.00	0.42
1:A:932:ASP:OD1	1:A:932:ASP:N	2.52	0.42
1:B:209:LEU:HB3	1:B:223:LEU:HD22	2.00	0.42
1:B:928:VAL:HG21	1:B:1173:ILE:CG2	2.45	0.42
1:D:1173:ILE:HG13	1:D:1231:LEU:HB2	2.01	0.42
1:A:98:ARG:HG3	1:A:644:ILE:HD13	2.01	0.42
1:A:950:LEU:HG	1:A:952:LEU:CD2	2.50	0.42
1:C:1191:THR:O	1:C:1191:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:ARG:HG2	1:D:738:PHE:CZ	2.54	0.42
1:D:587:LYS:HG2	1:D:671:ASN:OD1	2.19	0.42
1:A:262:GLU:HG3	1:A:263:GLU:H	1.82	0.42
1:A:264:ILE:CG2	1:A:265:THR:N	2.75	0.42
1:A:657:ALA:O	1:A:660:ASP:HB2	2.20	0.42
1:A:918:ASN:O	1:A:922:PRO:HA	2.20	0.42
1:A:945:ASN:ND2	1:A:951:LYS:HB3	2.35	0.42
1:A:1152:ALA:CB	1:A:1173:ILE:HG22	2.49	0.42
1:C:152:HIS:CD2	1:C:704:HIS:CE1	2.90	0.42
1:C:270:PHE:HB3	1:C:321:ASP:O	2.19	0.42
1:C:326:GLU:O	1:C:326:GLU:HG2	2.19	0.42
1:C:357:VAL:HG12	1:C:361:ASN:HD21	1.85	0.42
1:C:833:GLN:O	1:C:835:PHE:N	2.53	0.42
1:C:890:ILE:CG2	1:C:891:GLU:N	2.82	0.42
1:D:537:TYR:N	1:D:559:TYR:HE1	2.17	0.42
1:D:941:VAL:HG13	1:D:950:LEU:HD12	2.02	0.42
1:D:1193:ILE:O	1:D:1195:LYS:N	2.51	0.42
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.91	0.42
1:A:690:LYS:HA	1:A:699:ASP:OD1	2.19	0.42
1:A:706:ILE:HG22	1:A:707:GLU:N	2.35	0.42
1:A:803:GLU:O	1:A:871:VAL:HG23	2.19	0.42
1:A:918:ASN:HA	1:A:944:TYR:CZ	2.55	0.42
1:B:152:HIS:HD2	1:B:704:HIS:HE1	1.63	0.42
1:C:185:ILE:O	1:C:189:ARG:HG2	2.20	0.42
1:C:795:TYR:HB3	1:C:801:LEU:HD22	2.01	0.42
1:D:209:LEU:HD23	1:D:212:LEU:HD12	2.02	0.42
1:D:746:LEU:HD12	1:D:769:LEU:HB3	2.01	0.42
1:A:534:THR:HG21	1:A:572:LYS:C	2.40	0.42
1:A:675:THR:HB	1:A:710:PHE:CE2	2.54	0.42
1:B:511:TRP:HH2	1:B:566:ARG:NH2	2.16	0.42
1:B:1123:GLU:OE1	1:B:1219:THR:N	2.50	0.42
1:C:102:PHE:HA	1:C:597:PRO:HG3	2.01	0.42
1:C:293:LEU:HD22	1:C:537:TYR:CD1	2.55	0.42
1:C:700:ILE:HG22	1:C:704:HIS:HB2	2.00	0.42
1:A:212:LEU:CD2	1:A:548:TYR:CD1	3.03	0.42
1:A:945:ASN:HD22	1:A:1143:LYS:H	1.66	0.42
1:B:897:LEU:HD23	1:B:897:LEU:HA	1.84	0.42
1:C:165:LYS:HB3	1:C:165:LYS:HZ3	1.85	0.42
1:C:1199:ILE:CG2	1:C:1200:GLN:N	2.82	0.42
1:D:578:ILE:O	1:D:578:ILE:HD12	2.20	0.42
1:A:887:ASN:ND2	1:A:1195:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:THR:HG23	1:B:341:TYR:CB	2.48	0.42
1:B:534:THR:O	1:B:536:ASN:N	2.53	0.42
1:C:729:LYS:HD3	1:C:733:SER:O	2.20	0.42
1:A:67:TYR:OH	1:A:226:GLU:OE2	2.33	0.41
1:A:152:HIS:CE1	1:A:708:ARG:HG2	2.55	0.41
1:A:717:ASN:OD1	1:A:717:ASN:N	2.53	0.41
1:B:43:CYS:HB2	1:B:64:ILE:CD1	2.50	0.41
1:B:949:ARG:HG2	1:B:949:ARG:NH1	2.34	0.41
1:C:36:MET:CE	1:C:68:ILE:HG12	2.50	0.41
1:D:219:HIS:HD2	1:D:254:ARG:HH11	1.68	0.41
1:D:398:LEU:HD12	1:D:398:LEU:HA	1.83	0.41
1:A:280:ASP:O	1:A:284:VAL:HG23	2.20	0.41
1:A:301:LEU:C	1:A:303:LYS:N	2.74	0.41
1:B:140:MET:HE2	1:B:140:MET:HA	2.02	0.41
1:B:335:PHE:CD1	1:B:335:PHE:C	2.90	0.41
1:B:506:GLU:CD	1:B:506:GLU:H	2.23	0.41
1:B:514:GLN:O	1:B:518:ASP:HB2	2.20	0.41
1:B:854:THR:HG22	1:B:855:LYS:HG3	2.01	0.41
1:B:876:ARG:HE	1:B:880:GLY:HA2	1.84	0.41
1:D:94:MET:O	1:D:98:ARG:HB2	2.21	0.41
1:D:394:VAL:HG22	1:D:418:PHE:CE2	2.54	0.41
1:A:377:ARG:O	1:A:378:MET:C	2.57	0.41
1:A:830:ARG:HG3	1:A:831:LYS:O	2.20	0.41
1:B:252:ILE:HB	1:B:739:PRO:HG2	2.02	0.41
1:B:703:ASN:O	1:B:705:CYS:SG	2.67	0.41
1:B:1167:GLY:O	1:B:1186:THR:HG23	2.21	0.41
1:C:128:PHE:HE2	1:C:130:SER:HA	1.85	0.41
1:C:312:THR:CG2	1:C:338:TRP:NE1	2.81	0.41
1:C:918:ASN:HA	1:C:944:TYR:OH	2.20	0.41
1:D:58:GLU:OE1	1:D:695:GLY:HA3	2.20	0.41
1:D:358:GLU:HA	1:D:361:ASN:HD22	1.85	0.41
1:D:704:HIS:HE1	1:D:706:ILE:HG12	1.85	0.41
1:A:848:LYS:HB2	1:A:848:LYS:HE3	1.83	0.41
1:A:862:ILE:H	1:A:862:ILE:CD1	2.13	0.41
1:B:65:PHE:CE1	1:B:150:PHE:HB2	2.56	0.41
1:B:317:LEU:HD12	1:B:317:LEU:HA	1.83	0.41
1:B:962:GLU:CG	1:B:1169:ARG:HE	2.33	0.41
1:C:443:ILE:HD11	1:C:458:ASP:OD1	2.20	0.41
1:C:657:ALA:O	1:C:660:ASP:HB2	2.21	0.41
1:C:706:ILE:N	1:C:706:ILE:CD1	2.80	0.41
1:C:907:GLU:HA	1:C:910:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:929:PHE:HB2	1:C:939:ALA:HB2	2.01	0.41
1:D:155:ILE:HG22	1:D:706:ILE:HD12	2.01	0.41
1:D:565:PRO:HB2	1:D:566:ARG:H	1.64	0.41
1:D:881:SER:HB3	1:D:914:PRO:HD3	2.02	0.41
1:B:682:ASN:OD1	1:B:684:GLN:N	2.53	0.41
1:B:1118:SER:O	1:B:1122:VAL:HG23	2.20	0.41
1:C:250:LEU:O	1:C:254:ARG:HG3	2.20	0.41
1:C:514:GLN:HE21	1:C:517:LYS:HD2	1.84	0.41
1:C:787:LYS:HE3	1:C:787:LYS:HB2	1.96	0.41
1:C:918:ASN:HD22	1:C:918:ASN:N	2.17	0.41
1:D:294:PRO:HB2	1:D:564:ALA:HB2	2.02	0.41
1:B:12:GLU:OE1	1:B:762:SER:HB2	2.21	0.41
1:B:207:ALA:O	1:B:209:LEU:N	2.54	0.41
1:B:797:ARG:O	1:B:798:TRP:C	2.57	0.41
1:C:152:HIS:HA	1:C:706:ILE:CG1	2.41	0.41
1:C:592:LEU:HA	1:C:592:LEU:HD23	1.81	0.41
1:C:593:MET:HE1	1:C:604:ILE:HD12	2.03	0.41
1:D:599:ARG:HH22	1:D:625:ASN:HD21	1.68	0.41
1:A:10:ILE:HG21	1:A:10:ILE:HD13	1.50	0.41
1:A:768:VAL:HG13	1:A:858:LEU:HD13	2.02	0.41
1:A:1223:LEU:HD12	1:A:1223:LEU:HA	1.87	0.41
1:B:5:LYS:HD2	1:B:5:LYS:HA	1.89	0.41
1:B:264:ILE:CG2	1:B:265:THR:H	2.31	0.41
1:B:330:ILE:HD12	1:B:542:GLN:HG2	2.02	0.41
1:B:458:ASP:OD1	1:B:461:SER:HB3	2.19	0.41
1:C:917:ILE:CG1	1:C:947:GLU:O	2.69	0.41
1:C:1111:SER:HB3	1:C:1191:THR:HA	2.02	0.41
1:D:87:GLY:O	1:D:135:PRO:HG3	2.19	0.41
1:D:412:ASP:C	1:D:414:ASP:N	2.74	0.41
1:D:928:VAL:HG21	1:D:1173:ILE:CG2	2.48	0.41
1:D:934:ALA:HB2	1:D:956:LYS:HB3	2.00	0.41
1:D:952:LEU:CD2	1:D:1149:ILE:HD13	2.51	0.41
1:D:1192:SER:O	1:D:1194:GLY:N	2.54	0.41
1:A:212:LEU:HD21	1:A:548:TYR:CE1	2.56	0.41
1:A:855:LYS:HB2	1:A:857:ILE:HG13	2.03	0.41
1:B:155:ILE:HB	1:B:706:ILE:HD12	2.01	0.41
1:B:297:PRO:CG	1:B:298:ASP:H	2.34	0.41
1:B:301:LEU:HD22	1:B:306:PHE:CE2	2.56	0.41
1:C:182:MET:HE2	1:C:182:MET:HA	2.02	0.41
1:C:391:ILE:H	1:C:391:ILE:HG13	1.69	0.41
1:D:934:ALA:CB	1:D:956:LYS:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:O	1:A:113:GLN:N	2.54	0.41
1:A:391:ILE:HG13	1:A:391:ILE:H	1.68	0.41
1:A:685:VAL:HG21	1:A:707:GLU:OE2	2.20	0.41
1:A:831:LYS:H	1:A:831:LYS:CD	2.28	0.41
1:A:1207:ILE:HG22	1:A:1209:ALA:H	1.86	0.41
1:B:45:HIS:CE1	1:B:130:SER:HB2	2.56	0.41
1:B:159:THR:HA	1:B:162:GLN:HG2	2.02	0.41
1:B:366:ASN:O	1:B:367:ILE:C	2.58	0.41
1:B:864:ALA:O	1:B:895:LEU:N	2.47	0.41
1:B:1104:PHE:HB2	1:B:1106:VAL:HG23	2.03	0.41
1:B:1188:VAL:CG1	1:B:1202:LEU:HB2	2.50	0.41
1:B:1206:GLU:HA	1:B:1221:ARG:HG2	2.02	0.41
1:C:99:ALA:HB1	1:C:642:VAL:HG12	2.02	0.41
1:C:254:ARG:HH11	1:C:254:ARG:HD3	1.72	0.41
1:C:575:ASP:O	1:C:576:GLN:HB3	2.21	0.41
1:D:221:PHE:CB	1:D:250:LEU:HD12	2.48	0.41
1:D:387:GLN:CG	1:D:432:PHE:CZ	3.04	0.41
1:D:545:LEU:HA	1:D:545:LEU:HD22	1.80	0.41
1:D:707:GLU:N	1:D:707:GLU:OE1	2.52	0.41
1:A:355:ILE:O	1:A:355:ILE:HD12	2.21	0.41
1:A:862:ILE:N	1:A:862:ILE:CD1	2.80	0.41
1:A:965:ILE:O	1:A:966:GLY:C	2.58	0.41
1:A:1127:ILE:HG12	1:A:1221:ARG:NH2	2.35	0.41
1:B:44:THR:HG22	1:B:45:HIS:CE1	2.57	0.41
1:B:1210:GLY:C	1:B:1220:ARG:HG3	2.42	0.41
1:C:357:VAL:O	1:C:361:ASN:ND2	2.52	0.41
1:C:867:LYS:HE2	1:C:890:ILE:HD13	2.02	0.41
1:A:34:LEU:CD2	1:A:203:TYR:HB3	2.51	0.40
1:A:96:GLN:O	1:A:100:ARG:HG3	2.21	0.40
1:A:173:VAL:HA	1:A:174:PRO:HD3	1.89	0.40
1:A:744:LEU:HB2	1:A:798:TRP:HE1	1.85	0.40
1:A:941:VAL:HG13	1:A:950:LEU:HD12	2.02	0.40
1:B:376:THR:O	1:B:380:LYS:HG3	2.21	0.40
1:B:459:LEU:O	1:B:460:ASP:C	2.60	0.40
1:B:710:PHE:CE2	1:B:711:ILE:O	2.74	0.40
1:C:3:ILE:HB	1:C:6:PHE:HB2	2.04	0.40
1:C:359:TRP:HZ2	1:C:363:GLN:NE2	2.18	0.40
1:D:798:TRP:CG	1:D:799:PRO:N	2.88	0.40
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.94	0.40
1:A:708:ARG:HB2	1:A:708:ARG:NH1	2.35	0.40
1:A:840:PHE:O	1:A:844:LYS:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TYR:OH	1:B:200:HIS:CD2	2.75	0.40
1:C:536:ASN:HD22	1:C:536:ASN:HA	1.69	0.40
1:C:918:ASN:HD22	1:C:918:ASN:H	1.69	0.40
1:C:952:LEU:HD21	1:C:1149:ILE:HD13	2.03	0.40
1:D:81:PHE:O	1:D:166:VAL:HA	2.21	0.40
1:D:269:GLN:HB2	1:D:320:MET:O	2.21	0.40
1:D:391:ILE:HG13	1:D:392:GLY:N	2.36	0.40
1:A:201:CYS:HA	1:A:222:CYS:O	2.21	0.40
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.78	0.40
1:A:519:LYS:HD3	1:A:563:TYR:CE1	2.57	0.40
1:A:527:THR:HB	1:A:528:ASP:H	1.50	0.40
1:A:657:ALA:HA	1:A:660:ASP:HB2	2.03	0.40
1:A:676:ASP:CB	1:A:711:ILE:HG22	2.51	0.40
1:A:1156:TYR:O	1:A:1160:ARG:HG3	2.22	0.40
1:B:65:PHE:CZ	1:B:150:PHE:HB2	2.56	0.40
1:C:264:ILE:CG2	1:C:268:VAL:CG1	2.86	0.40
1:D:226:GLU:H	1:D:226:GLU:HG2	1.68	0.40
1:D:1189:GLY:O	1:D:1200:GLN:HB2	2.22	0.40
1:A:31:ASN:HA	1:A:80:THR:O	2.21	0.40
1:A:516:TYR:OH	1:A:569:ASP:OD2	2.12	0.40
1:B:1039:UNK:O	1:B:1040:UNK:C	2.68	0.40
1:B:1213:PHE:HB3	1:B:1216:ARG:HH11	1.87	0.40
1:C:146:ASN:OD1	1:C:693:LEU:HG	2.20	0.40
1:C:815:VAL:CG1	1:C:830:ARG:HH11	2.33	0.40
1:C:1102:LYS:CB	1:C:1103:PRO:CD	2.95	0.40
1:C:1147:GLU:CD	1:C:1147:GLU:H	2.24	0.40
1:D:527:THR:CG2	1:D:528:ASP:H	2.08	0.40
1:D:586:PHE:HB3	1:D:590:GLN:HB2	2.04	0.40
1:D:848:LYS:O	1:D:852:GLN:HG3	2.21	0.40
1:D:1226:ASP:HB3	1:D:1229:PHE:CE1	2.56	0.40
1:A:308:VAL:HG11	1:A:363:GLN:HG2	2.04	0.40
1:B:303:LYS:HZ2	1:B:357:VAL:H	1.69	0.40
1:B:458:ASP:OD1	1:B:461:SER:HB2	2.21	0.40
1:B:656:MET:O	1:B:659:TYR:HB2	2.22	0.40
1:C:104:THR:HG22	1:C:104:THR:O	2.21	0.40
1:C:152:HIS:HD2	1:C:704:HIS:HE1	1.62	0.40
1:C:862:ILE:H	1:C:862:ILE:CD1	2.29	0.40
1:C:1089:ILE:O	1:C:1090:LEU:C	2.59	0.40
1:D:16:GLN:HE22	1:D:799:PRO:HG3	1.87	0.40
1:D:907:GLU:H	1:D:907:GLU:HG2	1.70	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	1001/1155 (87%)	869 (87%)	95 (10%)	37 (4%)	3 13
1	B	998/1155 (86%)	842 (84%)	109 (11%)	47 (5%)	2 8
1	C	1008/1155 (87%)	866 (86%)	104 (10%)	38 (4%)	3 13
1	D	982/1155 (85%)	824 (84%)	117 (12%)	41 (4%)	3 10
All	All	3989/4620 (86%)	3401 (85%)	425 (11%)	163 (4%)	3 11

All (163) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ALA
1	A	112	LEU
1	A	263	GLU
1	A	265	THR
1	A	353	LYS
1	A	527	THR
1	A	528	ASP
1	A	607	VAL
1	A	702	HIS
1	A	712	PRO
1	A	798	TRP
1	A	799	PRO
1	A	861	ASP
1	A	1093	VAL
1	B	4	PRO
1	B	109	GLU
1	B	297	PRO
1	B	527	THR
1	B	596	LEU
1	B	701	GLU
1	B	712	PRO
1	B	716	GLU

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Mol	Chain	Res	Type
1	B	798	TRP
1	B	946	SER
1	B	1193	ILE
1	B	1235	ASP
1	C	111	ALA
1	C	112	LEU
1	C	113	GLN
1	C	428	ALA
1	C	606	VAL
1	C	607	VAL
1	C	702	HIS
1	C	712	PRO
1	C	834	ASP
1	C	860	ASP
1	C	1105	VAL
1	C	1138	GLN
1	D	264	ILE
1	D	267	SER
1	D	565	PRO
1	D	702	HIS
1	D	712	PRO
1	D	716	GLU
1	D	860	ASP
1	D	1193	ILE
1	D	1194	GLY
1	D	1236	ARG
1	A	92	ALA
1	A	193	ASP
1	A	518	ASP
1	A	596	LEU
1	A	713	GLU
1	A	754	SER
1	A	1095	ASP
1	B	56	SER
1	B	264	ILE
1	B	404	ARG
1	B	460	ASP
1	B	565	PRO
1	B	582	LYS
1	B	646	PHE
1	B	713	GLU
1	B	717	ASN

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Mol	Chain	Res	Type
1	B	822	GLY
1	B	981	PRO
1	B	1108	SER
1	B	1138	GLN
1	B	1139	LYS
1	B	1213	PHE
1	C	403	GLN
1	C	513	ASP
1	C	528	ASP
1	C	713	GLU
1	C	797	ARG
1	C	833	GLN
1	C	1104	PHE
1	C	1107	VAL
1	D	92	ALA
1	D	106	MET
1	D	269	GLN
1	D	303	LYS
1	D	582	LYS
1	D	624	PRO
1	D	713	GLU
1	A	191	GLN
1	A	302	LYS
1	A	461	SER
1	A	735	LEU
1	A	863	SER
1	A	917	ILE
1	A	1116	LYS
1	B	353	LYS
1	B	535	GLU
1	B	823	LYS
1	B	824	LEU
1	C	698	ASN
1	C	716	GLU
1	C	832	PRO
1	C	980	TYR
1	D	4	PRO
1	D	356	ASP
1	D	596	LEU
1	D	602	ASN
1	D	605	PRO
1	D	625	ASN

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Mol	Chain	Res	Type
1	D	701	GLU
1	D	714	SER
1	D	1112	ASP
1	D	1195	LYS
1	A	695	GLY
1	A	791	GLY
1	A	1111	SER
1	B	265	THR
1	B	602	ASN
1	B	624	PRO
1	B	649	GLN
1	B	774	LEU
1	B	812	GLU
1	B	972	LEU
1	B	1195	LYS
1	C	576	GLN
1	C	798	TRP
1	D	438	PHE
1	D	547	TYR
1	D	588	PRO
1	D	736	ALA
1	D	798	TRP
1	D	963	PRO
1	D	1143	LYS
1	A	605	PRO
1	A	606	VAL
1	B	106	MET
1	B	687	THR
1	B	861	ASP
1	C	4	PRO
1	C	413	ALA
1	C	714	SER
1	C	957	GLY
1	C	1208	ILE
1	D	265	THR
1	D	606	VAL
1	D	645	SER
1	A	113	GLN
1	A	664	SER
1	B	110	LYS
1	B	208	ASP
1	C	835	PHE

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Mol	Chain	Res	Type
1	C	1106	VAL
1	C	1194	GLY
1	A	264	ILE
1	B	653	VAL
1	B	1194	GLY
1	D	395	LYS
1	A	395	LYS
1	B	538	VAL
1	C	133	ILE
1	C	862	ILE
1	D	133	ILE
1	D	607	VAL
1	C	917	ILE
1	C	1103	PRO
1	D	553	PRO

5.3.2 Protein sidechains (i)

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	922/1004 (92%)	805 (87%)	117 (13%)	4 13
1	B	919/1004 (92%)	791 (86%)	128 (14%)	3 10
1	C	927/1004 (92%)	814 (88%)	113 (12%)	5 15
1	D	905/1004 (90%)	765 (84%)	140 (16%)	2 8
All	All	3673/4016 (92%)	3175 (86%)	498 (14%)	3 11

All (498) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	24	SER
1	A	36	MET
1	A	55	LEU
1	A	57	GLU
1	A	63	LYS

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Mol	Chain	Res	Type
1	A	96	GLN
1	A	98	ARG
1	A	112	LEU
1	A	113	GLN
1	A	114	LYS
1	A	137	THR
1	A	138	GLU
1	A	150	PHE
1	A	160	ARG
1	A	183	ASP
1	A	186	ARG
1	A	192	GLU
1	A	255	GLU
1	A	263	GLU
1	A	273	ASP
1	A	291	ASP
1	A	302	LYS
1	A	303	LYS
1	A	306	PHE
1	A	315	GLU
1	A	325	ASN
1	A	326	GLU
1	A	340	LYS
1	A	350	PHE
1	A	351	GLU
1	A	353	LYS
1	A	354	ASP
1	A	363	GLN
1	A	387	GLN
1	A	391	ILE
1	A	405	LYS
1	A	414	ASP
1	A	417	ILE
1	A	421	GLU
1	A	462	ILE
1	A	518	ASP
1	A	527	THR
1	A	534	THR
1	A	535	GLU
1	A	536	ASN
1	A	571	ILE
1	A	584	GLN

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Mol	Chain	Res	Type
1	A	587	LYS
1	A	590	GLN
1	A	591	GLN
1	A	602	ASN
1	A	641	VAL
1	A	645	SER
1	A	660	ASP
1	A	702	HIS
1	A	706	ILE
1	A	708	ARG
1	A	710	PHE
1	A	711	ILE
1	A	717	ASN
1	A	735	LEU
1	A	744	LEU
1	A	749	GLU
1	A	759	ASN
1	A	767	MET
1	A	773	ASP
1	A	781	SER
1	A	785	LEU
1	A	793	ILE
1	A	796	SER
1	A	802	ARG
1	A	810	ILE
1	A	816	TYR
1	A	819	VAL
1	A	829	GLU
1	A	831	LYS
1	A	846	THR
1	A	852	GLN
1	A	862	ILE
1	A	876	ARG
1	A	904	ASN
1	A	917	ILE
1	A	918	ASN
1	A	932	ASP
1	A	948	THR
1	A	951	LYS
1	A	952	LEU
1	A	962	GLU
1	A	965	ILE

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Mol	Chain	Res	Type
1	A	978	ARG
1	A	982	THR
1	A	983	GLN
1	A	1091	LYS
1	A	1093	VAL
1	A	1095	ASP
1	A	1098	SER
1	A	1107	VAL
1	A	1110	GLU
1	A	1112	ASP
1	A	1113	SER
1	A	1119	MET
1	A	1140	LYS
1	A	1141	LEU
1	A	1143	LYS
1	A	1147	GLU
1	A	1149	ILE
1	A	1150	LEU
1	A	1153	GLU
1	A	1173	ILE
1	A	1178	LYS
1	A	1191	THR
1	A	1196	ASN
1	A	1216	ARG
1	A	1221	ARG
1	A	1232	ASN
1	A	1239	VAL
1	B	4	PRO
1	B	10	ILE
1	B	25	GLN
1	B	55	LEU
1	B	57	GLU
1	B	59	GLU
1	B	62	SER
1	B	63	LYS
1	B	67	TYR
1	B	83	MET
1	B	96	GLN
1	B	112	LEU
1	B	113	GLN
1	B	114	LYS
1	B	130	SER

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Mol	Chain	Res	Type
1	B	131	ASN
1	B	149	TYR
1	B	159	THR
1	B	182	MET
1	B	183	ASP
1	B	189	ARG
1	B	195	ASN
1	B	226	GLU
1	B	228	VAL
1	B	252	ILE
1	B	263	GLU
1	B	271	GLU
1	B	290	ASN
1	B	306	PHE
1	B	315	GLU
1	B	325	ASN
1	B	332	LEU
1	B	335	PHE
1	B	340	LYS
1	B	350	PHE
1	B	355	ILE
1	B	370	GLU
1	B	383	LEU
1	B	386	GLN
1	B	391	ILE
1	B	395	LYS
1	B	402	VAL
1	B	404	ARG
1	B	407	THR
1	B	417	ILE
1	B	449	SER
1	B	460	ASP
1	B	462	ILE
1	B	506	GLU
1	B	513	ASP
1	B	514	GLN
1	B	518	ASP
1	B	527	THR
1	B	529	SER
1	B	531	LYS
1	B	542	GLN
1	B	571	ILE

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Mol	Chain	Res	Type
1	B	576	GLN
1	B	578	ILE
1	B	591	GLN
1	B	602	ASN
1	B	606	VAL
1	B	622	PHE
1	B	651	ARG
1	B	669	LYS
1	B	684	GLN
1	B	691	THR
1	B	703	ASN
1	B	706	ILE
1	B	707	GLU
1	B	710	PHE
1	B	711	ILE
1	B	713	GLU
1	B	725	PRO
1	B	735	LEU
1	B	754	SER
1	B	765	GLN
1	B	772	GLN
1	B	774	LEU
1	B	813	GLU
1	B	819	VAL
1	B	821	SER
1	B	825	THR
1	B	828	ILE
1	B	831	LYS
1	B	843	LEU
1	B	850	ASN
1	B	852	GLN
1	B	853	ARG
1	B	854	THR
1	B	858	LEU
1	B	860	ASP
1	B	879	ASP
1	B	889	THR
1	B	902	VAL
1	B	903	LYS
1	B	917	ILE
1	B	918	ASN
1	B	932	ASP

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Mol	Chain	Res	Type
1	B	956	LYS
1	B	965	ILE
1	B	974	SER
1	B	978	ARG
1	B	979	PHE
1	B	980	TYR
1	B	983	GLN
1	B	1093	VAL
1	B	1097	LEU
1	B	1098	SER
1	B	1109	LEU
1	B	1110	GLU
1	B	1112	ASP
1	B	1113	SER
1	B	1116	LYS
1	B	1118	SER
1	B	1128	LYS
1	B	1130	VAL
1	B	1139	LYS
1	B	1143	LYS
1	B	1149	ILE
1	B	1153	GLU
1	B	1163	ARG
1	B	1178	LYS
1	B	1191	THR
1	B	1192	SER
1	B	1196	ASN
1	B	1232	ASN
1	B	1239	VAL
1	C	4	PRO
1	C	10	ILE
1	C	17	ILE
1	C	26	ILE
1	C	38	SER
1	C	44	THR
1	C	54	ARG
1	C	55	LEU
1	C	58	GLU
1	C	59	GLU
1	C	62	SER
1	C	67	TYR
1	C	98	ARG

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Mol	Chain	Res	Type
1	C	101	ARG
1	C	113	GLN
1	C	137	THR
1	C	140	MET
1	C	143	LEU
1	C	154	LYS
1	C	176	GLU
1	C	183	ASP
1	C	189	ARG
1	C	195	ASN
1	C	226	GLU
1	C	290	ASN
1	C	303	LYS
1	C	306	PHE
1	C	317	LEU
1	C	320	MET
1	C	321	ASP
1	C	339	LEU
1	C	351	GLU
1	C	354	ASP
1	C	355	ILE
1	C	357	VAL
1	C	376	THR
1	C	383	LEU
1	C	389	LYS
1	C	402	VAL
1	C	412	ASP
1	C	417	ILE
1	C	427	ARG
1	C	435	GLU
1	C	447	SER
1	C	449	SER
1	C	513	ASP
1	C	515	TYR
1	C	518	ASP
1	C	526	ASP
1	C	528	ASP
1	C	530	LEU
1	C	531	LYS
1	C	532	GLU
1	C	536	ASN
1	C	545	LEU

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Mol	Chain	Res	Type
1	C	591	GLN
1	C	600	SER
1	C	604	ILE
1	C	606	VAL
1	C	621	ASP
1	C	641	VAL
1	C	642	VAL
1	C	643	LYS
1	C	650	LYS
1	C	666	ASP
1	C	675	THR
1	C	699	ASP
1	C	701	GLU
1	C	707	GLU
1	C	708	ARG
1	C	710	PHE
1	C	711	ILE
1	C	715	MET
1	C	730	LEU
1	C	735	LEU
1	C	764	GLN
1	C	772	GLN
1	C	782	LEU
1	C	810	ILE
1	C	814	THR
1	C	823	LYS
1	C	824	LEU
1	C	826	LYS
1	C	830	ARG
1	C	833	GLN
1	C	836	GLU
1	C	841	ARG
1	C	842	GLU
1	C	852	GLN
1	C	858	LEU
1	C	861	ASP
1	C	883	SER
1	C	887	ASN
1	C	907	GLU
1	C	917	ILE
1	C	918	ASN
1	C	923	LYS

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Mol	Chain	Res	Type
1	C	932	ASP
1	C	948	THR
1	C	952	LEU
1	C	969	ARG
1	C	977	LEU
1	C	1088	SER
1	C	1097	LEU
1	C	1107	VAL
1	C	1109	LEU
1	C	1149	ILE
1	C	1155	SER
1	C	1178	LYS
1	C	1192	SER
1	C	1232	ASN
1	C	1236	ARG
1	C	1239	VAL
1	D	4	PRO
1	D	10	ILE
1	D	26	ILE
1	D	31	ASN
1	D	42	ASN
1	D	58	GLU
1	D	66	SER
1	D	67	TYR
1	D	98	ARG
1	D	113	GLN
1	D	154	LYS
1	D	155	ILE
1	D	160	ARG
1	D	164	VAL
1	D	186	ARG
1	D	195	ASN
1	D	221	PHE
1	D	226	GLU
1	D	228	VAL
1	D	248	LEU
1	D	262	GLU
1	D	265	THR
1	D	266	ASP
1	D	268	VAL
1	D	280	ASP
1	D	291	ASP

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Mol	Chain	Res	Type
1	D	293	LEU
1	D	306	PHE
1	D	315	GLU
1	D	325	ASN
1	D	329	LYS
1	D	339	LEU
1	D	340	LYS
1	D	352	LYS
1	D	353	LYS
1	D	354	ASP
1	D	358	GLU
1	D	363	GLN
1	D	378	MET
1	D	383	LEU
1	D	387	GLN
1	D	389	LYS
1	D	400	LYS
1	D	402	VAL
1	D	405	LYS
1	D	406	VAL
1	D	412	ASP
1	D	417	ILE
1	D	423	LYS
1	D	427	ARG
1	D	438	PHE
1	D	440	LEU
1	D	448	LYS
1	D	449	SER
1	D	459	LEU
1	D	462	ILE
1	D	510	GLU
1	D	513	ASP
1	D	532	GLU
1	D	536	ASN
1	D	542	GLN
1	D	545	LEU
1	D	550	ARG
1	D	556	SER
1	D	574	ILE
1	D	575	ASP
1	D	579	GLU
1	D	580	PHE

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Mol	Chain	Res	Type
1	D	593	MET
1	D	596	LEU
1	D	601	LYS
1	D	606	VAL
1	D	607	VAL
1	D	608	TYR
1	D	625	ASN
1	D	662	LYS
1	D	672	SER
1	D	679	PHE
1	D	703	ASN
1	D	706	ILE
1	D	707	GLU
1	D	709	GLU
1	D	710	PHE
1	D	711	ILE
1	D	713	GLU
1	D	715	MET
1	D	718	VAL
1	D	719	LYS
1	D	730	LEU
1	D	735	LEU
1	D	743	THR
1	D	746	LEU
1	D	747	THR
1	D	764	GLN
1	D	772	GLN
1	D	774	LEU
1	D	784	ASP
1	D	797	ARG
1	D	813	GLU
1	D	820	LYS
1	D	821	SER
1	D	825	THR
1	D	826	LYS
1	D	835	PHE
1	D	838	LYS
1	D	839	GLU
1	D	843	LEU
1	D	844	LYS
1	D	845	MET
1	D	863	SER

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Mol	Chain	Res	Type
1	D	876	ARG
1	D	879	ASP
1	D	917	ILE
1	D	918	ASN
1	D	926	LYS
1	D	946	SER
1	D	948	THR
1	D	949	ARG
1	D	950	LEU
1	D	952	LEU
1	D	962	GLU
1	D	964	ASN
1	D	968	VAL
1	D	969	ARG
1	D	972	LEU
1	D	977	LEU
1	D	1128	LYS
1	D	1130	VAL
1	D	1136	SER
1	D	1138	GLN
1	D	1140	LYS
1	D	1143	LYS
1	D	1147	GLU
1	D	1149	ILE
1	D	1150	LEU
1	D	1155	SER
1	D	1175	ASP
1	D	1195	LYS
1	D	1232	ASN
1	D	1239	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	25	GLN
1	A	41	HIS
1	A	96	GLN
1	A	97	GLN
1	A	113	GLN
1	A	152	HIS
1	A	195	ASN

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Mol	Chain	Res	Type
1	A	200	HIS
1	A	219	HIS
1	A	220	HIS
1	A	311	GLN
1	A	319	HIS
1	A	325	ASN
1	A	327	GLN
1	A	362	GLN
1	A	363	GLN
1	A	366	ASN
1	A	386	GLN
1	A	387	GLN
1	A	446	HIS
1	A	649	GLN
1	A	759	ASN
1	A	770	HIS
1	A	850	ASN
1	A	918	ASN
1	A	945	ASN
1	A	983	GLN
1	A	1196	ASN
1	A	1232	ASN
1	B	16	GLN
1	B	19	GLN
1	B	96	GLN
1	B	113	GLN
1	B	152	HIS
1	B	195	ASN
1	B	200	HIS
1	B	219	HIS
1	B	220	HIS
1	B	290	ASN
1	B	319	HIS
1	B	325	ASN
1	B	327	GLN
1	B	386	GLN
1	B	576	GLN
1	B	591	GLN
1	B	684	GLN
1	B	702	HIS
1	B	887	ASN
1	B	918	ASN

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Mol	Chain	Res	Type
1	B	945	ASN
1	B	964	ASN
1	B	975	GLN
1	B	1196	ASN
1	B	1232	ASN
1	C	16	GLN
1	C	19	GLN
1	C	25	GLN
1	C	96	GLN
1	C	97	GLN
1	C	152	HIS
1	C	195	ASN
1	C	200	HIS
1	C	219	HIS
1	C	220	HIS
1	C	269	GLN
1	C	290	ASN
1	C	319	HIS
1	C	325	ASN
1	C	387	GLN
1	C	429	ASN
1	C	446	HIS
1	C	514	GLN
1	C	590	GLN
1	C	591	GLN
1	C	759	ASN
1	C	770	HIS
1	C	850	ASN
1	C	852	GLN
1	C	904	ASN
1	C	918	ASN
1	C	945	ASN
1	C	975	GLN
1	C	1138	GLN
1	C	1232	ASN
1	D	16	GLN
1	D	25	GLN
1	D	73	HIS
1	D	97	GLN
1	D	152	HIS
1	D	157	ASN
1	D	179	HIS

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Mol	Chain	Res	Type
1	D	195	ASN
1	D	200	HIS
1	D	219	HIS
1	D	220	HIS
1	D	295	ASN
1	D	300	HIS
1	D	325	ASN
1	D	361	ASN
1	D	363	GLN
1	D	403	GLN
1	D	446	HIS
1	D	576	GLN
1	D	590	GLN
1	D	591	GLN
1	D	625	ASN
1	D	702	HIS
1	D	703	ASN
1	D	753	ASN
1	D	770	HIS
1	D	904	ASN
1	D	918	ASN
1	D	945	ASN
1	D	964	ASN
1	D	1212	ASN
1	D	1232	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1023/1155 (88%)	-0.31	11 (1%)	80	80	34, 57, 89, 110	0
1	B	1020/1155 (88%)	-0.23	21 (2%)	63	61	29, 64, 116, 133	0
1	C	1030/1155 (89%)	-0.18	20 (1%)	66	65	32, 72, 100, 124	0
1	D	1004/1155 (86%)	-0.08	23 (2%)	60	58	43, 79, 123, 144	0
All	All	4077/4620 (88%)	-0.20	75 (1%)	68	67	29, 67, 113, 144	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	663	LEU	5.7
1	A	229	THR	5.0
1	D	229	THR	4.8
1	D	399	LEU	3.9
1	B	717	ASN	3.7
1	D	408	SER	3.6
1	B	641	VAL	3.6
1	D	319	HIS	3.3
1	D	112	LEU	3.3
1	A	983	GLN	3.2
1	A	46	GLY	3.2
1	B	577	ASN	3.2
1	A	115	ALA	3.1
1	C	1083	SER	3.1
1	A	702	HIS	3.1
1	A	112	LEU	3.1
1	D	504	TYR	3.1
1	C	1086	ALA	3.0
1	C	310	LEU	3.0
1	D	284	VAL	2.9
1	D	106	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	511	TRP	2.8
1	D	979	PHE	2.8
1	B	112	LEU	2.8
1	A	351	GLU	2.7
1	B	284	VAL	2.7
1	B	108	ALA	2.7
1	C	981	PRO	2.6
1	B	662	LYS	2.6
1	B	106	MET	2.6
1	C	1097	LEU	2.6
1	B	643	LYS	2.5
1	B	718	VAL	2.5
1	C	687	THR	2.5
1	C	309	LEU	2.5
1	A	662	LYS	2.5
1	C	284	VAL	2.5
1	C	229	THR	2.5
1	D	662	LYS	2.4
1	C	1104	PHE	2.4
1	B	663	LEU	2.4
1	B	703	ASN	2.4
1	B	661	ALA	2.4
1	D	576	GLN	2.4
1	A	284	VAL	2.3
1	B	281	PHE	2.3
1	C	823	LYS	2.3
1	D	981	PRO	2.3
1	C	111	ALA	2.3
1	D	515	TYR	2.2
1	C	703	ASN	2.2
1	B	312	THR	2.2
1	C	1133	PRO	2.2
1	C	312	THR	2.2
1	D	823	LYS	2.2
1	D	608	TYR	2.2
1	B	665	PRO	2.2
1	D	1107	VAL	2.2
1	B	111	ALA	2.2
1	D	111	ALA	2.2
1	B	649	GLN	2.2
1	C	313	PHE	2.2
1	C	112	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	1192	SER	2.1
1	A	717	ASN	2.1
1	C	1196	ASN	2.1
1	A	799	PRO	2.1
1	C	717	ASN	2.1
1	B	608	TYR	2.1
1	B	820	LYS	2.1
1	D	379	GLY	2.1
1	D	703	ASN	2.1
1	D	375	ARG	2.0
1	C	702	HIS	2.0
1	D	110	LYS	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.