Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2018 – 05:48 pm GMT

PDB ID	:	3FFZ
Title	:	Domain organization in Clostridium butulinum neurotoxin type E is unique: Its implication in faster translocation
Authors	:	Kumaran, D.; Eswaramoorthy, S.; Swaminathan, S.
Deposited on	:	2008-12-04
Resolution	:	2.65 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 following versions of software and data (see references (i)) were used in the production of this report:

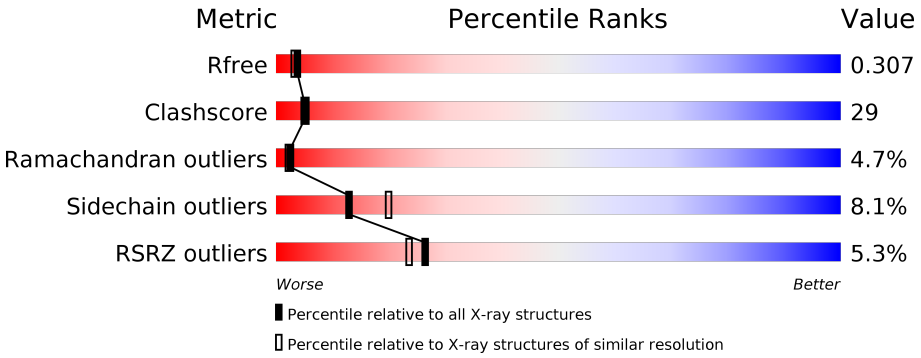
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

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 2.65 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}	111664	1112 (2.68-2.64)
Clashscore	122126	1151 (2.68-2.64)
Ramachandran outliers	120053	1133 (2.68-2.64)
Sidechain outliers	120020	1133 (2.68-2.64)
RSRZ outliers	108989	1098 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1252	4% 53% 39% 7%
1	B	1252	6% 47% 45% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	1301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20217 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 Botulinum neurotoxin type E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1246	Total	C	N	O	S	0	0	0
			10085	6414	1686	1961	24			
1	B	1238	Total	C	N	O	S	0	0	0
			10025	6375	1674	1952	24			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLY	ARG	SEE REMARK 999	UNP Q00496
A	340	ALA	ARG	SEE REMARK 999	UNP Q00496
A	963	LEU	PHE	SEE REMARK 999	UNP Q00496
A	964	GLN	GLU	SEE REMARK 999	UNP Q00496
A	967	ALA	ARG	SEE REMARK 999	UNP Q00496
A	1195	ASN	-	INSERTION	UNP Q00496
B	177	GLY	ARG	SEE REMARK 999	UNP Q00496
B	340	ALA	ARG	SEE REMARK 999	UNP Q00496
B	963	LEU	PHE	SEE REMARK 999	UNP Q00496
B	964	GLN	GLU	SEE REMARK 999	UNP Q00496
B	967	ALA	ARG	SEE REMARK 999	UNP Q00496
B	1195	ASN	-	INSERTION	UNP Q00496

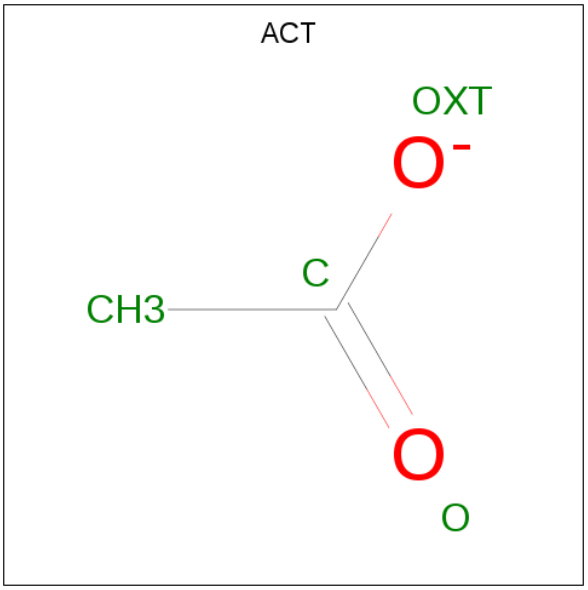
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	2	Total Na 2 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

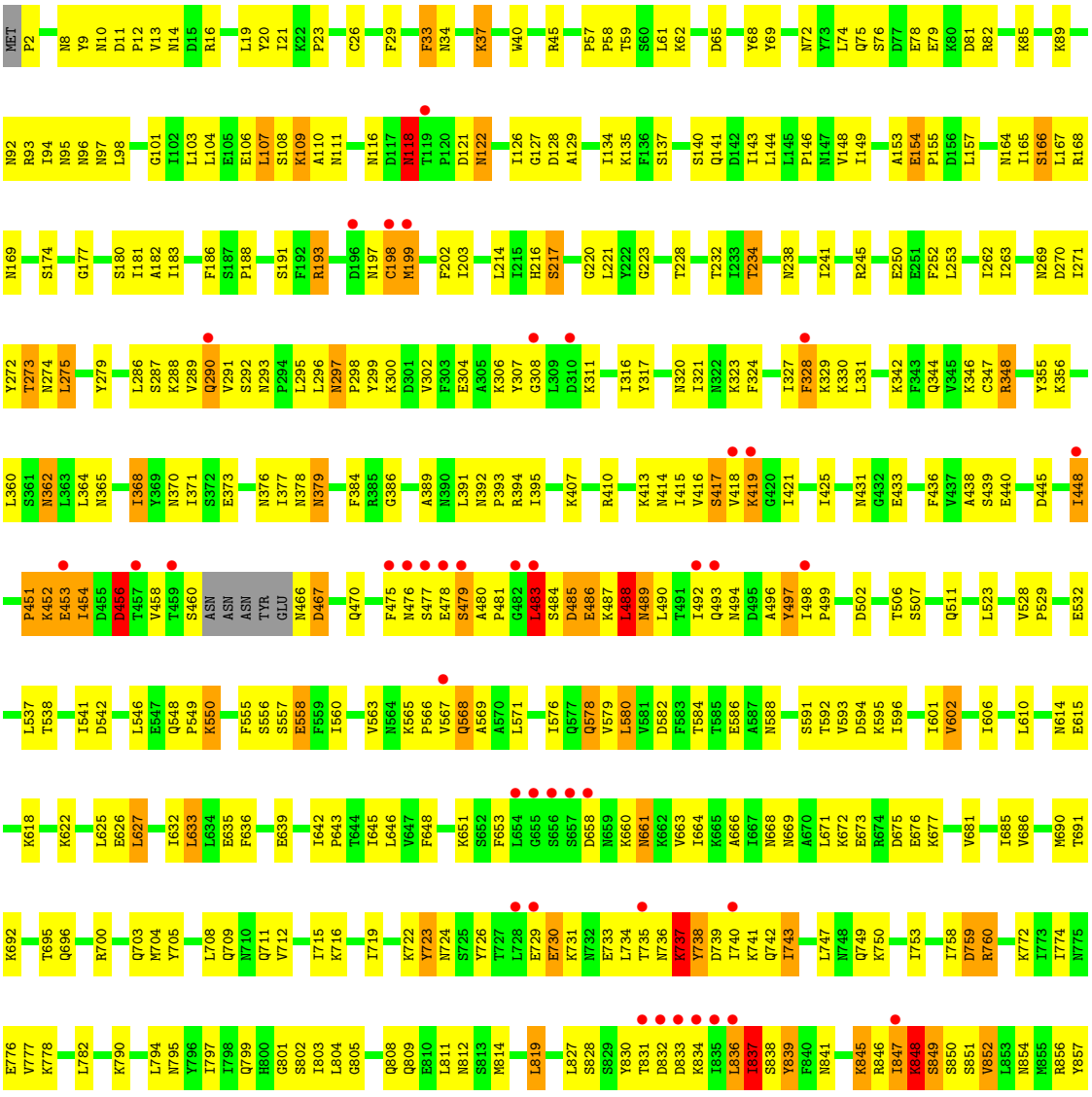
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	62	Total O 62 62	0	0
5	B	32	Total O 32 32	0	0

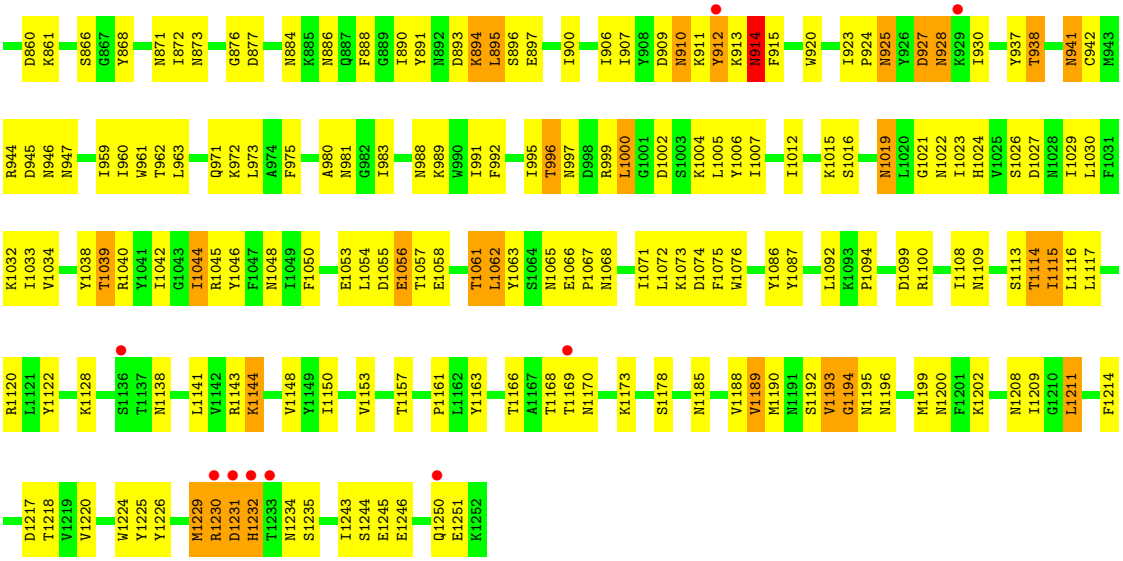
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 geometryand 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: Botulinum neurotoxin type E

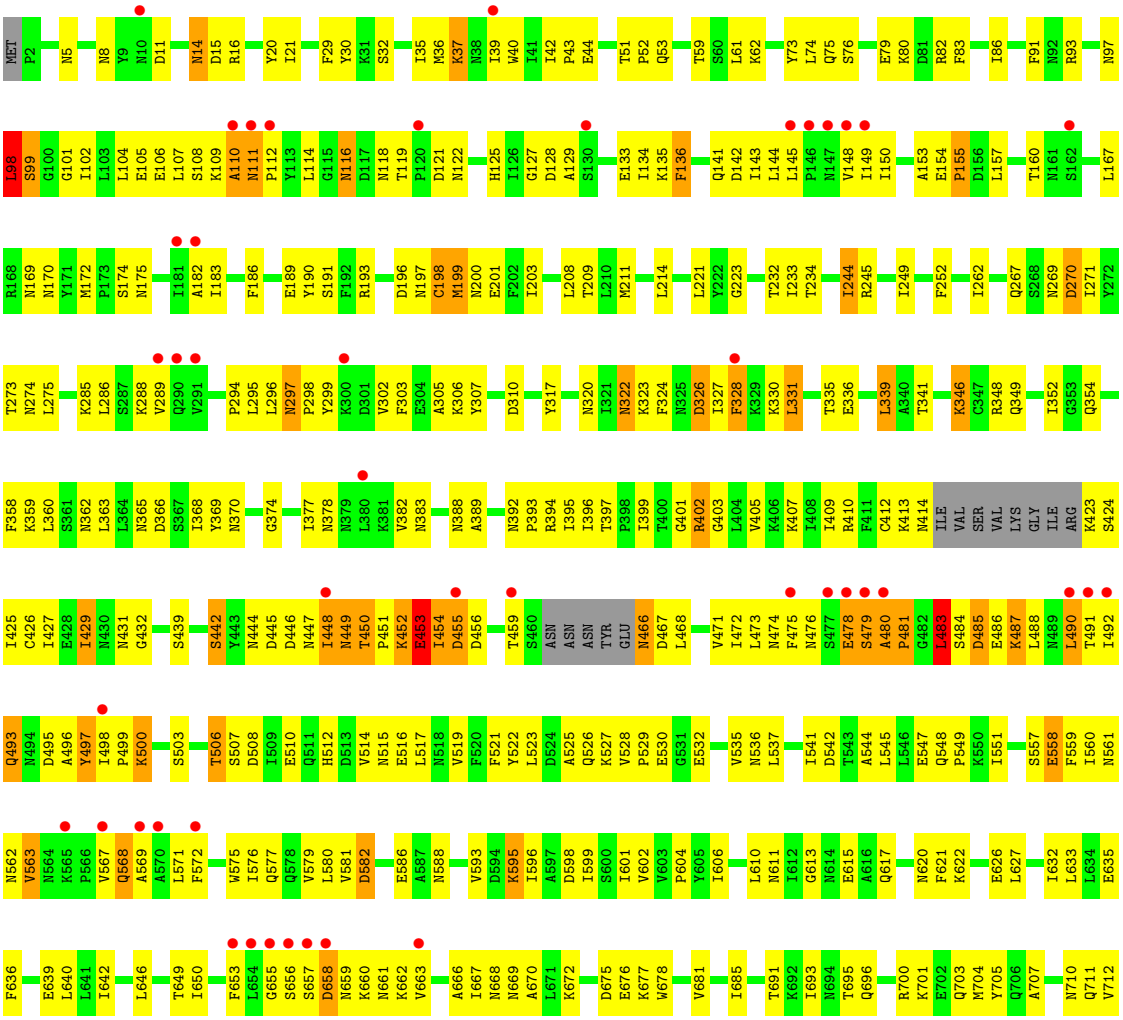
Chain A:

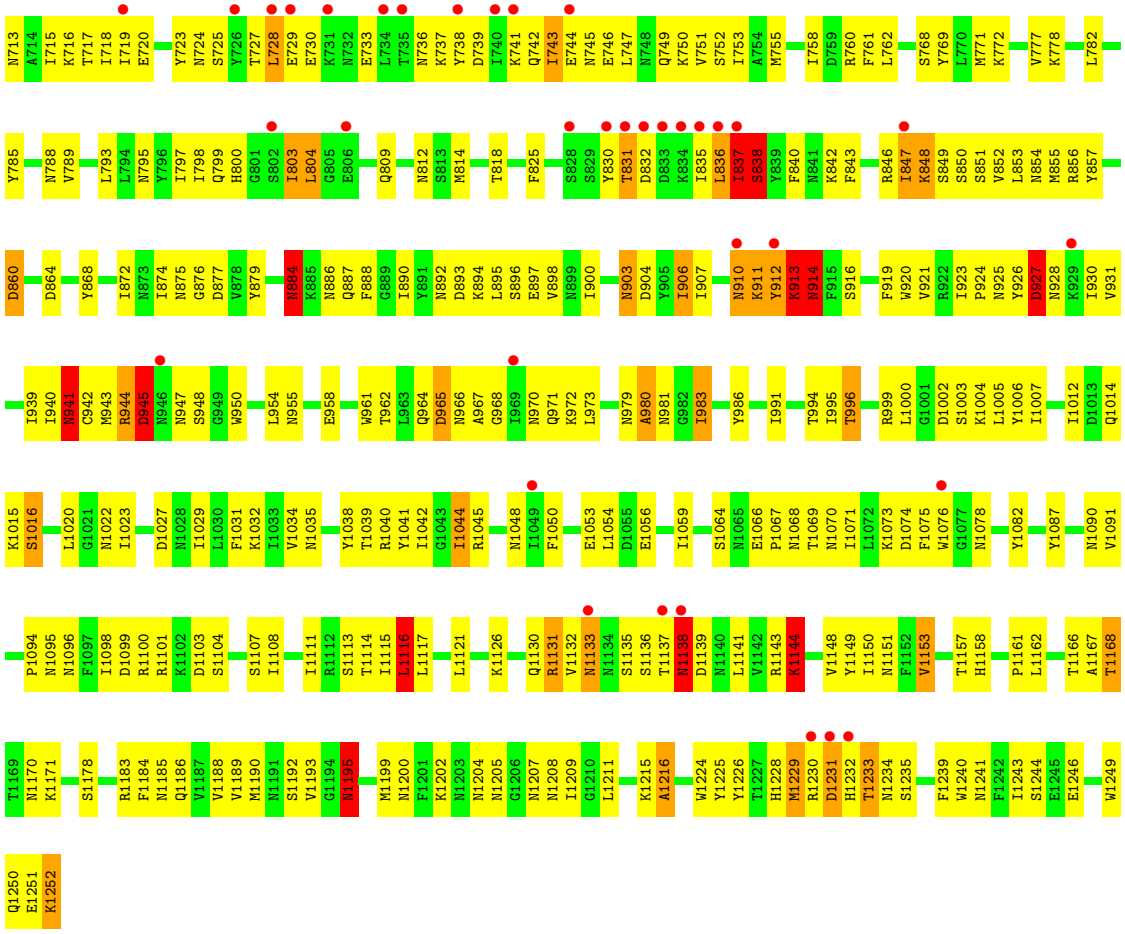




• Molecule 1: Botulinum neurotoxin type E

Chain B:




N713 A714 I715 K716 T717 I718 I719 E720
Y723 N724 S725 Y726 T727 L728 E729 E730 K731 N732 E733 L734 T735 N736 K737 Y738 D739 I740 K741 Q742 I743 E744 N745 E746 L747 N748 Q749 K750 V751 S752 I753 A754 M755
I758 D759 R760 F761 L762
S768 Y769 L770 M771 K772
V777 K778
L782
Y785 N788 V789 L793 L794 N795 Y796 I797 I798 Q799 H800 G801 S802 I803 L804 G805 E806 Q809 N812 S813 M814 T818 F825 S828 S829 Y830 T831 D832 D833 K834 I835 L836 I837 S838 Y839 F840 N841 K842 F843 R846 I847 K848 S849 S850 S851 V852 L853 N854 M855 R856 Y857
D860 D864 Y868 I872 N873 I874 N875 G876 D877 V878 Y879 N884 K885 N886 Q887 F888 G889 I890 Y891 N892 D893 K894 L895 S896 E897 V898 N899 I900 N903 D904 Y905 I906 I907 N910 K911 Y912 K913 N914 F915 S916 F919 W920 V921 R922 I923 P924 N925 Y926 D927 N928 K929 I930 V931
I939 I940 N941 C942 M943 R944 D945 N946 N947 S948 G949 W950 L954 N955 E958 W961 T962 L963 Q964 D965 N966 A967 G968 I969 N970 Q971 K972 L973 N979 A980 N981 G982 I983 Y986 I991 T994 I995 T996 R999 L1000 G1001 D1002 S1003 K1004 L1005 Y1006 I1007 I1012 D1013 Q1014
K1015 S1016 L1020 G1021 N1022 I1023 D1027 N1028 I1029 L1030 F1031 K1032 I1033 V1034 N1035 Y1038 T1039 R1040 Y1041 I1042 G1043 I1044 R1045 N1048 I1049 F1050 E1053 L1054 D1055 E1056 I1059 S1064 N1065 E1066 P1067 N1068 T1069 N1070 I1071 L1072 K1073 D1074 F1075 W1076 G1077 N1078 Y1082 Y1087 N1090 V1091
P1094 N1095 N1096 F1097 I1098 D1099 R1100 R1101 K1102 D1103 S1104 S1107 I1108 I1111 R1112 S1113 T1114 I1115 L1116 L1117 L1121 K1126 Q1130 R1131 V1132 N1133 N1134 S1135 S1136 T1137 N1138 D1139 N1140 L1141 V1142 R1143 K1144 V1148 Y1149 I1150 N1151 F1152 V1153 T1157 H1158 P1161 L1162 T1166 A1167 T1168
T1169 N1170 K1171 S1178 R1183 F1184 N1185 Q1186 V1187 V1188 V1189 M1190 N1191 S1192 V1193 G1194 N1195 M1199 N1200 F1201 K1202 N1203 N1204 N1205 G1206 N1207 N1208 I1209 G1210 L1211 K1215 A1216 W1224 Y1225 Y1226 T1227 H1228 M1229 R1230 D1231 H1232 T1233 N1234 S1235 F1239 W1240 N1241 F1242 I1243 S1244 E1245 E1246 W1249
Q1250 E1251 K1252

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.43Å 172.57Å 137.26Å 90.00° 99.84° 90.00°	Depositor
Resolution (Å)	29.49 – 2.65 33.84 – 2.49	Depositor EDS
% Data completeness (in resolution range)	86.5 (29.49-2.65) 75.9 (33.84-2.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.309 0.252 , 0.307	Depositor DCC
R_{free} test set	4751 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	20217	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.24% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, ACT

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	0.47	0/10285	0.73	4/13934 (0.0%)
1	B	0.43	1/10224 (0.0%)	0.71	8/13851 (0.1%)
All	All	0.45	1/20509 (0.0%)	0.72	12/27785 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	449	ASN	C-N	6.70	1.49	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	450	THR	C-N-CD	-14.63	88.41	120.60
1	B	1138	ASN	C-N-CA	6.99	139.17	121.70
1	B	1232	HIS	N-CA-C	6.39	128.25	111.00
1	A	914	ASN	N-CA-C	6.16	127.63	111.00
1	A	483	LEU	N-CA-C	6.13	127.56	111.00
1	B	655	GLY	N-CA-C	-6.09	97.89	113.10
1	B	1195	ASN	N-CA-C	-5.95	94.93	111.00
1	A	488	LEU	N-CA-C	5.56	126.02	111.00
1	B	1116	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	848	LYS	N-CA-C	-5.13	97.16	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1144	LYS	N-CA-C	5.08	124.72	111.00
1	B	836	LEU	N-CA-C	-5.08	97.29	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1138	ASN	Mainchain

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	10085	0	9924	533	0
1	B	10025	0	9849	624	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	2	0
3	B	1	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	62	0	0	10	0
5	B	32	0	0	1	0
All	All	20217	0	19779	1158	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 29.

All (1158) 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:B:448:ILE:CG1	1:B:646:LEU:HG	1.80	1.10
1:A:914:ASN:ND2	1:A:914:ASN:H	1.42	1.09
1:A:852:VAL:HG13	1:A:906:ILE:HD12	1.35	1.08
1:A:568:GLN:HG3	1:A:571:LEU:HD22	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ILE:HG13	1:B:646:LEU:HG	1.34	1.05
1:B:109:LYS:HE3	1:B:479:SER:HB2	1.39	1.03
1:B:660:LYS:HG2	1:B:804:LEU:HB3	1.42	1.00
1:A:568:GLN:HB2	1:A:571:LEU:HD13	1.42	0.98
1:A:448:ILE:CG2	1:A:646:LEU:HG	1.93	0.98
1:A:297:ASN:H	1:A:298:PRO:HD2	1.27	0.97
3:A:1301:NA:NA	5:A:1317:HOH:O	1.34	0.97
1:B:606:ILE:HG12	1:B:704:MET:HE3	1.46	0.96
1:B:448:ILE:HG12	1:B:646:LEU:CD1	1.96	0.95
1:A:448:ILE:HG23	1:A:646:LEU:H	1.32	0.94
1:A:238:ASN:HB3	1:A:241:ILE:HG12	1.50	0.93
1:A:856:ARG:HH21	1:A:1048:ASN:HD21	1.16	0.92
1:B:1190:MET:CE	1:B:1199:MET:HG2	2.00	0.92
1:A:944:ARG:HG2	1:A:1026:SER:HB2	1.51	0.92
1:B:996:THR:HG23	1:B:1053:GLU:HG2	1.52	0.91
1:B:1130:GLN:NE2	1:B:1151:ASN:HD21	1.69	0.91
1:A:914:ASN:N	1:A:914:ASN:HD22	1.59	0.90
1:A:1057:THR:O	1:A:1061:THR:HG22	1.71	0.90
1:A:836:LEU:HD12	1:A:837:ILE:H	1.37	0.90
1:B:197:ASN:HD21	1:B:346:LYS:HD3	1.34	0.89
1:B:884:ASN:HD21	1:B:886:ASN:HB2	1.37	0.89
1:A:417:SER:OG	1:A:421:ILE:HB	1.73	0.89
1:A:857:TYR:H	1:A:886:ASN:HD21	1.17	0.88
1:B:498:ILE:O	1:B:498:ILE:HG13	1.73	0.88
1:B:297:ASN:H	1:B:298:PRO:HD2	1.37	0.88
1:A:448:ILE:HD11	1:A:643:PRO:HG2	1.56	0.87
1:B:742:GLN:HB3	1:B:743:ILE:HD12	1.57	0.86
1:A:635:GLU:H	1:A:696:GLN:NE2	1.74	0.85
1:B:295:LEU:HD23	1:B:488:LEU:HD13	1.58	0.85
1:B:295:LEU:HD12	1:B:295:LEU:H	1.40	0.85
1:B:981:ASN:HB3	1:B:1117:LEU:HB3	1.57	0.84
1:B:448:ILE:CG1	1:B:646:LEU:CG	2.55	0.83
1:A:302:VAL:HG23	1:A:483:LEU:HD22	1.60	0.83
1:B:983:ILE:HD12	1:B:983:ILE:H	1.43	0.82
1:A:448:ILE:HD12	1:A:645:ILE:HA	1.61	0.82
1:A:857:TYR:H	1:A:886:ASN:ND2	1.76	0.82
1:B:1190:MET:HE1	1:B:1199:MET:HG2	1.61	0.82
1:B:1137:THR:HG22	1:B:1137:THR:O	1.77	0.82
1:A:197:ASN:O	1:A:198:CYS:HB2	1.79	0.82
1:B:448:ILE:HG12	1:B:646:LEU:HD12	1.62	0.82
1:A:660:LYS:HB2	1:A:803:ILE:HG22	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:ASN:N	1:A:1019:ASN:HD22	1.76	0.81
1:A:996:THR:HG22	1:A:1004:LYS:HB2	1.62	0.81
1:A:297:ASN:H	1:A:298:PRO:CD	1.93	0.81
1:B:1130:GLN:HE21	1:B:1151:ASN:HD21	1.22	0.81
1:A:475:PHE:HB2	1:A:1143:ARG:HD3	1.61	0.81
1:A:292:SER:HB2	1:A:296:LEU:HD11	1.62	0.80
1:A:833:ASP:CB	1:A:836:LEU:HD23	2.10	0.80
1:A:636:PHE:H	1:A:696:GLN:HE22	1.30	0.80
1:A:914:ASN:H	1:A:914:ASN:HD22	0.80	0.80
1:B:642:ILE:HD11	1:B:685:ILE:HD11	1.63	0.80
1:B:275:LEU:HD23	1:B:328:PHE:CE1	2.16	0.79
1:B:448:ILE:CD1	1:B:646:LEU:HG	2.11	0.79
1:A:180:SER:O	1:A:221:LEU:HD23	1.82	0.79
1:A:454:ILE:HG13	1:A:666:ALA:HB1	1.62	0.79
1:A:615:GLU:H	1:A:615:GLU:CD	1.84	0.79
1:A:606:ILE:HG23	1:A:704:MET:HE1	1.64	0.79
1:B:453:GLU:OE1	1:B:453:GLU:HA	1.82	0.79
1:B:632:ILE:HG23	1:B:633:LEU:HD22	1.63	0.79
1:A:847:ILE:HD12	1:A:847:ILE:H	1.46	0.78
1:A:448:ILE:HG21	1:A:646:LEU:HG	1.65	0.78
1:B:294:PRO:HG2	1:B:295:LEU:HD12	1.65	0.78
1:B:410:ARG:HD2	1:B:426:CYS:SG	2.23	0.78
1:A:1019:ASN:H	1:A:1019:ASN:HD22	1.27	0.78
1:B:579:VAL:HG23	1:B:580:LEU:HD23	1.64	0.78
1:A:451:PRO:HG2	1:A:648:PHE:HB3	1.65	0.77
1:B:999:ARG:HH11	1:B:999:ARG:HA	1.48	0.77
1:A:925:ASN:C	1:A:927:ASP:H	1.82	0.77
1:B:487:LYS:HD2	1:B:487:LYS:O	1.85	0.77
1:A:203:ILE:HD11	1:A:389:ALA:HB2	1.67	0.77
1:A:914:ASN:ND2	1:A:914:ASN:N	2.21	0.77
1:B:109:LYS:HA	1:B:483:LEU:HG	1.65	0.76
1:B:814:MET:O	1:B:818:THR:HG23	1.83	0.76
1:A:593:VAL:HG23	1:A:602:VAL:HG22	1.68	0.76
1:A:893:ASP:HB3	1:A:1039:THR:HG22	1.67	0.76
1:A:1211:LEU:HD13	1:A:1226:TYR:HE2	1.50	0.76
1:B:354:GLN:HG2	1:B:432:GLY:HA2	1.68	0.76
1:B:837:ILE:O	1:B:838:SER:HB3	1.86	0.76
1:A:1190:MET:CE	1:A:1199:MET:HG2	2.16	0.76
1:A:961:TRP:CE3	1:A:995:ILE:HD13	2.20	0.76
1:B:536:ASN:C	1:B:537:LEU:HD12	2.07	0.75
1:B:116:ASN:HD22	1:B:118:ASN:H	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:ASN:HB3	1:A:1117:LEU:HD23	1.69	0.75
1:B:148:VAL:HG22	1:B:182:ALA:HB3	1.69	0.75
1:B:875:ASN:HB2	1:B:897:GLU:HB2	1.69	0.75
1:A:836:LEU:CD1	1:A:837:ILE:H	1.98	0.75
1:A:972:LYS:O	1:A:1015:LYS:HE2	1.86	0.74
1:A:410:ARG:HB3	1:A:511:GLN:HG3	1.67	0.74
1:B:738:TYR:HA	1:B:743:ILE:HD13	1.69	0.74
1:A:109:LYS:HA	1:A:483:LEU:HD11	1.69	0.74
1:A:356:LYS:HD3	5:A:1283:HOH:O	1.87	0.74
1:B:1251:GLU:HG2	1:B:1252:LYS:H	1.53	0.74
1:B:111:ASN:HD22	1:B:483:LEU:HD12	1.52	0.74
1:B:944:ARG:HD3	1:B:945:ASP:N	2.02	0.74
1:B:856:ARG:HH21	1:B:1048:ASN:HD22	1.35	0.74
1:A:484:SER:O	1:A:485:ASP:HB2	1.88	0.73
1:B:76:SER:HB3	1:B:79:GLU:HB2	1.70	0.73
1:A:391:LEU:C	1:A:393:PRO:HD3	2.09	0.73
1:A:1006:TYR:HE2	1:A:1056:GLU:HG2	1.54	0.73
1:B:448:ILE:HG13	1:B:646:LEU:CG	2.15	0.73
1:A:448:ILE:HG22	1:A:646:LEU:CG	2.18	0.73
1:B:857:TYR:CZ	1:B:860:ASP:HA	2.24	0.73
1:A:373:GLU:HB2	1:A:377:ILE:HG22	1.68	0.73
1:A:379:ASN:N	1:A:379:ASN:HD22	1.86	0.73
1:A:910:ASN:OD1	1:A:912:TYR:HB3	1.88	0.73
1:B:93:ARG:HH11	1:B:93:ARG:HG3	1.51	0.73
1:A:379:ASN:H	1:A:379:ASN:HD22	1.35	0.73
1:B:925:ASN:C	1:B:927:ASP:H	1.91	0.73
1:B:1135:SER:O	1:B:1138:ASN:HB2	1.89	0.73
1:A:29:PHE:CE1	1:A:135:LYS:HG3	2.24	0.72
1:B:1116:LEU:HD12	5:B:1255:HOH:O	1.88	0.72
1:A:480:ALA:HB3	1:A:481:PRO:HD3	1.71	0.72
1:B:466:ASN:N	1:B:466:ASN:HD22	1.87	0.72
1:A:165:ILE:CD1	1:A:181:ILE:HB	2.20	0.72
1:A:851:SER:HB3	1:A:854:ASN:HD21	1.54	0.72
1:B:1188:VAL:HG21	1:B:1199:MET:HB3	1.71	0.72
1:B:715:ILE:O	1:B:718:ILE:HG22	1.89	0.72
1:A:856:ARG:NH2	1:A:1048:ASN:HD21	1.85	0.72
1:A:203:ILE:CD1	1:A:389:ALA:HB2	2.20	0.72
1:B:297:ASN:H	1:B:298:PRO:CD	2.02	0.72
1:B:529:PRO:HG3	1:B:548:GLN:O	1.89	0.72
1:A:550:LYS:O	3:A:1301:NA:NA	1.61	0.72
1:A:448:ILE:HG22	1:A:646:LEU:HG	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:LEU:HD22	1:A:563:VAL:HG11	1.71	0.72
1:A:467:ASP:HB3	1:A:470:GLN:HB3	1.73	0.71
1:B:1161:PRO:HG2	1:B:1178:SER:HB3	1.71	0.71
1:B:448:ILE:CG1	1:B:646:LEU:CD1	2.68	0.71
1:A:1092:LEU:O	1:A:1094:PRO:HD3	1.90	0.71
1:A:269:ASN:O	1:A:273:THR:HG22	1.90	0.71
1:B:1002:ASP:HA	1:B:1016:SER:HA	1.73	0.71
1:B:98:LEU:HD12	1:B:472:ILE:HG23	1.73	0.71
1:A:913:LYS:HB3	1:A:914:ASN:ND2	2.06	0.71
1:A:1076:TRP:HZ3	1:A:1244:SER:O	1.73	0.70
1:B:962:THR:HG22	1:B:972:LYS:HG2	1.72	0.70
1:B:907:ILE:HD13	1:B:1027:ASP:HA	1.73	0.70
1:B:560:ILE:O	1:B:563:VAL:HG12	1.92	0.70
1:A:454:ILE:HG21	1:A:666:ALA:HB2	1.72	0.70
1:B:99:SER:HB3	1:B:472:ILE:HD11	1.74	0.70
1:A:20:TYR:HB3	1:A:29:PHE:HB3	1.74	0.70
1:A:910:ASN:CG	1:A:912:TYR:HB3	2.11	0.69
1:B:1252:LYS:HE3	1:B:1252:LYS:HA	1.74	0.69
1:B:109:LYS:CE	1:B:479:SER:HB2	2.19	0.69
1:A:941:ASN:HD22	1:A:942:CYS:N	1.90	0.69
1:B:299:TYR:HA	1:B:302:VAL:HG12	1.74	0.69
1:B:425:ILE:HD13	1:B:545:LEU:HB3	1.74	0.69
1:B:944:ARG:HH11	1:B:944:ARG:HA	1.58	0.69
1:B:211:MET:HA	1:B:214:LEU:HD12	1.73	0.69
1:B:642:ILE:HD13	1:B:681:VAL:HG13	1.74	0.69
1:A:529:PRO:HG2	1:A:532:GLU:HG3	1.74	0.69
1:A:711:GLN:O	1:A:715:ILE:HG12	1.93	0.69
1:A:1148:VAL:O	1:A:1188:VAL:HG12	1.93	0.69
1:B:577:GLN:O	1:B:581:VAL:HG23	1.94	0.68
1:A:1076:TRP:CZ3	1:A:1244:SER:O	2.46	0.68
1:B:199:MET:HG2	1:B:705:TYR:CE2	2.28	0.68
1:A:944:ARG:HG2	1:A:1026:SER:CB	2.22	0.68
1:B:835:ILE:CG2	1:B:837:ILE:HB	2.22	0.68
1:A:122:ASN:HA	1:A:289:VAL:HA	1.75	0.68
1:A:448:ILE:CG2	1:A:646:LEU:CG	2.70	0.68
1:B:110:ALA:HB3	1:B:221:LEU:HD13	1.75	0.68
1:B:1074:ASP:HB2	1:B:1078:ASN:H	1.59	0.68
1:B:877:ASP:O	1:B:896:SER:HB2	1.93	0.68
1:A:127:GLY:HA2	1:A:493:GLN:NE2	2.08	0.68
1:A:1225:TYR:O	1:A:1229:MET:HB3	1.94	0.68
1:B:111:ASN:HD21	1:B:484:SER:HB2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1202:LYS:HA	1:B:1209:ILE:HG12	1.75	0.67
1:B:20:TYR:HB3	1:B:29:PHE:HB3	1.76	0.67
1:B:622:LYS:O	1:B:626:GLU:HG2	1.93	0.67
1:A:365:ASN:O	1:A:368:ILE:HG22	1.94	0.67
1:B:466:ASN:N	1:B:466:ASN:ND2	2.40	0.67
1:A:141:GLN:HE21	1:A:490:LEU:HD23	1.59	0.67
1:A:297:ASN:N	1:A:298:PRO:HD2	2.07	0.67
1:A:568:GLN:CB	1:A:571:LEU:HD13	2.22	0.67
1:B:51:THR:HG22	1:B:52:PRO:HD2	1.76	0.67
1:B:672:LYS:O	1:B:675:ASP:HB2	1.95	0.67
1:B:21:ILE:HG12	1:B:134:ILE:HG22	1.77	0.66
1:A:925:ASN:C	1:A:927:ASP:N	2.49	0.66
1:A:451:PRO:HG2	1:A:648:PHE:CB	2.26	0.66
1:A:57:PRO:HB3	1:A:69:TYR:HB2	1.76	0.66
1:A:663:VAL:HG21	1:A:804:LEU:HD23	1.77	0.66
1:B:474:ASN:HD22	1:B:1070:ASN:HB2	1.59	0.66
1:B:999:ARG:HH11	1:B:999:ARG:CA	2.07	0.66
1:A:606:ILE:HG23	1:A:704:MET:CE	2.25	0.66
1:A:857:TYR:N	1:A:886:ASN:ND2	2.44	0.66
1:B:884:ASN:ND2	1:B:886:ASN:HB2	2.10	0.66
1:B:368:ILE:HG12	1:B:395:ILE:HG22	1.78	0.65
1:A:116:ASN:HD21	1:A:118:ASN:HB2	1.61	0.65
1:B:835:ILE:HG22	1:B:837:ILE:HB	1.77	0.65
1:A:111:ASN:HD22	1:A:483:LEU:HD13	1.61	0.65
1:A:857:TYR:N	1:A:886:ASN:HD21	1.93	0.65
1:B:414:ASN:OD1	1:B:424:SER:HB3	1.96	0.65
1:A:615:GLU:CD	1:A:615:GLU:N	2.50	0.65
1:A:94:ILE:HG22	1:A:104:LEU:HD11	1.79	0.65
1:B:964:GLN:HG3	1:B:970:ASN:HB3	1.79	0.65
1:A:296:LEU:O	1:A:296:LEU:HD12	1.96	0.65
1:B:981:ASN:HB3	1:B:1117:LEU:HD23	1.77	0.65
1:B:429:ILE:HD13	1:B:429:ILE:H	1.62	0.65
1:A:1230:ARG:O	1:A:1231:ASP:HB2	1.97	0.64
1:B:249:ILE:HA	1:B:252:PHE:HD1	1.62	0.64
1:B:29:PHE:CE1	1:B:135:LYS:HG3	2.32	0.64
1:B:448:ILE:HD11	1:B:646:LEU:HG	1.78	0.64
1:B:109:LYS:HD2	1:B:483:LEU:HD23	1.78	0.64
1:B:402:ARG:HE	1:B:402:ARG:HA	1.63	0.64
1:A:801:GLY:HA3	1:A:808:GLN:OE1	1.98	0.64
1:B:468:LEU:O	1:B:471:VAL:HG22	1.95	0.64
1:B:498:ILE:N	1:B:499:PRO:HD3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:LYS:HA	1:A:999:ARG:CG	2.27	0.64
1:B:941:ASN:HD22	1:B:941:ASN:N	1.94	0.64
1:A:154:GLU:HB2	1:A:155:PRO:CD	2.28	0.64
1:B:659:ASN:HB3	1:B:662:LYS:HG2	1.79	0.64
1:B:928:ASN:C	1:B:930:ILE:H	2.01	0.64
1:B:1229:MET:O	1:B:1229:MET:HG2	1.95	0.64
1:B:275:LEU:HD23	1:B:328:PHE:HE1	1.60	0.64
1:A:989:LYS:HE2	1:A:1075:PHE:O	1.96	0.64
1:A:700:ARG:HD3	1:A:703:GLN:NE2	2.13	0.64
1:B:1095:ASN:C	1:B:1096:ASN:HD22	2.00	0.64
1:A:245:ARG:HH22	1:A:502:ASP:HB3	1.62	0.64
1:A:166:SER:HB3	1:A:498:ILE:HB	1.79	0.63
1:A:831:THR:O	1:A:831:THR:HG23	1.98	0.63
1:A:1092:LEU:C	1:A:1094:PRO:HD3	2.19	0.63
1:B:1167:ALA:O	1:B:1168:THR:HG23	1.98	0.63
1:B:903:ASN:HD22	1:B:904:ASP:N	1.96	0.63
1:B:996:THR:HG22	1:B:996:THR:O	1.99	0.63
1:B:931:VAL:HG13	1:B:1038:TYR:OH	1.98	0.63
1:A:1161:PRO:HG2	1:A:1178:SER:HB3	1.78	0.63
1:B:111:ASN:HD22	1:B:483:LEU:CD1	2.10	0.63
1:A:700:ARG:HD3	1:A:703:GLN:HE22	1.64	0.63
1:A:738:TYR:HA	1:A:743:ILE:HD13	1.81	0.63
1:A:778:LYS:HA	1:A:782:LEU:HB2	1.80	0.63
1:A:850:SER:O	1:A:1050:PHE:HA	1.99	0.63
1:A:1244:SER:O	1:A:1246:GLU:HG3	1.99	0.63
1:B:439:SER:O	1:B:442:SER:HB2	1.97	0.63
1:A:37:LYS:HA	1:A:37:LYS:HE3	1.80	0.63
1:A:1067:PRO:HA	5:A:1287:HOH:O	1.98	0.62
1:B:448:ILE:O	1:B:448:ILE:HG23	1.99	0.62
1:B:925:ASN:C	1:B:927:ASP:N	2.52	0.62
1:A:571:LEU:N	1:A:571:LEU:HD12	2.14	0.62
1:B:389:ALA:HA	1:B:396:ILE:HD11	1.81	0.62
1:B:749:GLN:O	1:B:753:ILE:HG12	1.98	0.62
1:B:1130:GLN:HE22	1:B:1183:ARG:HH22	1.46	0.62
1:B:197:ASN:ND2	1:B:346:LYS:HD3	2.12	0.62
1:A:642:ILE:HD13	1:A:681:VAL:HG13	1.81	0.62
1:B:746:GLU:O	1:B:750:LYS:HG2	1.99	0.62
1:B:1225:TYR:O	1:B:1229:MET:HB3	2.00	0.62
1:A:660:LYS:HG3	1:A:804:LEU:HA	1.81	0.62
1:A:833:ASP:HB3	1:A:836:LEU:HD23	1.82	0.62
1:A:92:ASN:O	1:A:96:ASN:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LYS:HE2	1:B:346:LYS:HA	1.81	0.61
1:A:847:ILE:N	1:A:847:ILE:HD12	2.14	0.61
1:B:606:ILE:HD12	1:B:761:PHE:HE2	1.64	0.61
1:B:831:THR:HG22	1:B:831:THR:O	2.00	0.61
1:B:169:ASN:O	1:B:170:ASN:HB2	2.01	0.61
1:B:62:LYS:O	1:B:407:LYS:HE3	2.00	0.61
1:B:580:LEU:HD22	1:B:747:LEU:HD21	1.81	0.61
1:B:704:MET:HG3	1:B:758:ILE:HD13	1.81	0.61
1:A:373:GLU:HB3	1:A:376:ASN:O	2.00	0.61
1:A:458:VAL:HG12	1:A:460:SER:H	1.66	0.61
1:A:719:ILE:HG22	1:A:719:ILE:O	2.01	0.61
1:A:238:ASN:HB3	1:A:241:ILE:CG1	2.29	0.61
1:B:378:ASN:HD22	1:B:378:ASN:N	1.98	0.61
1:A:116:ASN:ND2	1:A:118:ASN:HB2	2.15	0.61
1:A:895:LEU:HD12	1:A:895:LEU:N	2.16	0.60
1:B:1114:THR:CG2	1:B:1115:ILE:N	2.64	0.60
1:B:857:TYR:H	1:B:886:ASN:ND2	1.98	0.60
1:B:872:ILE:HG12	1:B:900:ILE:HG12	1.83	0.60
1:A:636:PHE:N	1:A:696:GLN:HE22	1.96	0.60
1:A:642:ILE:HD11	1:A:685:ILE:HD11	1.81	0.60
1:B:856:ARG:NH2	1:B:1048:ASN:HD22	1.99	0.60
1:B:955:ASN:HB3	1:B:958:GLU:CD	2.21	0.60
1:A:668:ASN:ND2	1:A:913:LYS:NZ	2.48	0.60
1:B:1171:LYS:NZ	1:B:1224:TRP:HB2	2.15	0.60
1:B:785:TYR:O	1:B:789:VAL:HG23	2.01	0.60
1:B:635:GLU:HB3	1:B:696:GLN:HE21	1.66	0.60
1:A:59:THR:HB	1:A:507:SER:HA	1.84	0.60
1:A:803:ILE:N	1:A:803:ILE:HD12	2.16	0.60
1:A:963:LEU:HD11	1:A:1023:ILE:HD13	1.82	0.60
1:A:1074:ASP:HB3	1:A:1076:TRP:H	1.67	0.60
1:A:593:VAL:HG23	1:A:602:VAL:CG2	2.32	0.60
1:A:742:GLN:CB	1:A:743:ILE:HD12	2.32	0.60
1:A:214:LEU:HA	1:A:217:SER:HB2	1.84	0.60
1:A:742:GLN:HB3	1:A:743:ILE:HD12	1.84	0.60
1:B:233:ILE:HD13	1:B:691:THR:HG21	1.84	0.60
1:B:848:LYS:O	1:B:848:LYS:HG3	2.01	0.60
1:A:454:ILE:HD12	1:A:666:ALA:HA	1.84	0.60
1:A:907:ILE:HD13	1:A:1027:ASP:HA	1.84	0.60
1:B:102:ILE:O	1:B:105:GLU:HB3	2.01	0.60
1:B:497:TYR:C	1:B:499:PRO:HD3	2.23	0.60
1:A:610:LEU:HD11	1:A:704:MET:HE2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:LYS:HA	1:A:999:ARG:HG3	1.83	0.60
1:B:174:SER:HA	1:B:223:GLY:HA2	1.84	0.60
1:B:795:ASN:O	1:B:799:GLN:HG2	2.02	0.60
1:B:847:ILE:O	1:B:848:LYS:HB3	2.02	0.60
1:A:1002:ASP:HB3	1:A:1016:SER:HA	1.83	0.59
1:A:854:ASN:HD22	1:A:866:SER:HA	1.66	0.59
1:B:1098:ILE:HD12	1:B:1098:ILE:N	2.17	0.59
1:A:216:HIS:CD2	5:A:1318:HOH:O	2.55	0.59
1:B:359:LYS:HB3	1:B:397:THR:HG23	1.83	0.59
1:B:668:ASN:HD21	1:B:913:LYS:HE2	1.67	0.59
1:B:928:ASN:CB	1:B:930:ILE:HD13	2.31	0.59
1:B:955:ASN:HB3	1:B:958:GLU:CG	2.33	0.59
1:A:1109:ASN:HB3	1:A:1217:ASP:HB2	1.85	0.59
1:A:228:THR:HB	1:A:250:GLU:HB2	1.84	0.59
1:B:128:ASP:HB2	1:B:495:ASP:O	2.03	0.59
1:B:532:GLU:OE2	1:B:549:PRO:HB3	2.02	0.59
1:A:342:LYS:HA	1:A:342:LYS:HE2	1.85	0.59
1:B:1132:VAL:HG23	1:B:1148:VAL:HA	1.83	0.59
1:B:269:ASN:O	1:B:273:THR:HG23	2.01	0.59
1:B:1130:GLN:NE2	1:B:1183:ARG:HH22	2.01	0.59
1:B:244:ILE:HG12	1:B:245:ARG:O	2.01	0.59
1:B:884:ASN:C	1:B:884:ASN:HD22	2.04	0.59
1:B:966:ASN:ND2	1:B:1022:ASN:HD22	2.01	0.59
1:B:642:ILE:CD1	1:B:685:ILE:HD11	2.32	0.59
1:A:595:LYS:HB2	1:A:626:GLU:HB2	1.84	0.59
1:B:874:ILE:O	1:B:874:ILE:HD12	2.03	0.59
1:B:947:ASN:HB3	1:B:964:GLN:HE22	1.67	0.59
1:A:576:ILE:O	1:A:580:LEU:HB2	2.03	0.59
1:B:37:LYS:HE3	1:B:37:LYS:HA	1.84	0.59
1:B:480:ALA:N	1:B:481:PRO:HD3	2.18	0.58
1:B:707:ALA:O	1:B:711:GLN:HG2	2.03	0.58
1:A:668:ASN:HD21	1:A:913:LYS:NZ	2.01	0.58
1:A:836:LEU:HD12	1:A:837:ILE:HD13	1.84	0.58
1:B:1006:TYR:O	1:B:1007:ILE:HD13	2.03	0.58
1:B:606:ILE:HD12	1:B:761:PHE:CE2	2.37	0.58
1:B:620:ASN:HD22	1:B:620:ASN:N	2.00	0.58
1:A:1150:ILE:HG12	1:A:1188:VAL:HG11	1.86	0.58
1:A:438:ALA:HB3	1:A:692:LYS:HG2	1.85	0.58
1:A:497:TYR:C	1:A:499:PRO:HD3	2.23	0.58
1:B:981:ASN:CB	1:B:1117:LEU:HB3	2.33	0.58
1:A:704:MET:HG3	1:A:758:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ASN:OD1	1:B:1039:THR:HA	2.03	0.58
1:B:1230:ARG:O	1:B:1231:ASP:HB2	2.03	0.58
1:B:852:VAL:HG13	1:B:906:ILE:CG1	2.34	0.58
1:A:362:ASN:HD21	1:A:364:LEU:HB2	1.69	0.58
1:B:836:LEU:O	1:B:837:ILE:HG22	2.04	0.58
1:B:837:ILE:O	1:B:838:SER:CB	2.51	0.58
1:A:368:ILE:HD11	1:A:395:ILE:HG22	1.84	0.58
1:B:193:ARG:HD2	1:B:201:GLU:HB3	1.86	0.58
1:A:498:ILE:O	1:A:498:ILE:HG12	2.04	0.58
1:B:660:LYS:HD3	1:B:660:LYS:O	2.04	0.58
1:A:1211:LEU:HD13	1:A:1226:TYR:CE2	2.36	0.58
1:A:368:ILE:O	1:A:368:ILE:HD13	2.03	0.58
1:A:448:ILE:CG2	1:A:646:LEU:H	2.14	0.58
1:A:959:ILE:C	1:A:960:ILE:HD12	2.25	0.57
1:B:1114:THR:HG21	1:B:1117:LEU:H	1.68	0.57
1:B:21:ILE:HG23	1:B:134:ILE:HG22	1.86	0.57
1:B:285:LYS:HB3	1:B:285:LYS:NZ	2.20	0.57
1:B:961:TRP:HD1	1:B:973:LEU:HB2	1.70	0.57
1:B:452:LYS:H	1:B:452:LYS:HD3	1.70	0.57
1:A:94:ILE:CG2	1:A:104:LEU:HD11	2.34	0.57
1:A:760:ARG:HE	1:A:830:TYR:HD2	1.50	0.57
1:B:755:MET:SD	1:B:758:ILE:HD12	2.44	0.57
1:B:913:LYS:HG3	1:B:914:ASN:H	1.69	0.57
1:B:1132:VAL:HG22	1:B:1149:TYR:CZ	2.39	0.57
1:B:106:GLU:CD	1:B:330:LYS:HD2	2.25	0.57
1:B:914:ASN:HB3	1:B:1053:GLU:HB2	1.86	0.57
1:A:989:LYS:HG2	1:A:1076:TRP:HA	1.87	0.57
1:A:376:ASN:HD22	1:A:386:GLY:HA3	1.70	0.57
1:A:836:LEU:HB3	1:A:837:ILE:HG12	1.86	0.57
1:B:1098:ILE:HA	1:B:1107:SER:O	2.04	0.57
1:B:480:ALA:N	1:B:481:PRO:CD	2.68	0.57
1:B:529:PRO:HG2	1:B:532:GLU:HB2	1.87	0.57
1:B:854:ASN:O	1:B:864:ASP:HA	2.03	0.57
1:B:947:ASN:HB3	1:B:964:GLN:NE2	2.18	0.57
1:A:938:THR:HG23	1:A:1034:VAL:HB	1.85	0.57
1:A:1062:LEU:O	1:A:1066:GLU:HG3	2.05	0.57
1:A:1202:LYS:HG2	1:A:1208:ASN:HA	1.87	0.57
1:A:760:ARG:HH21	1:A:831:THR:HG22	1.70	0.57
1:B:1132:VAL:HG22	1:B:1149:TYR:CE2	2.40	0.57
1:B:1190:MET:HE2	1:B:1199:MET:HG2	1.84	0.57
1:B:615:GLU:CD	1:B:615:GLU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1200:ASN:HB2	1:B:1211:LEU:HD12	1.86	0.56
1:B:134:ILE:HD13	1:B:144:LEU:HB2	1.87	0.56
1:A:1071:ILE:O	1:A:1073:LYS:HE3	2.05	0.56
1:B:1114:THR:HG22	1:B:1115:ILE:N	2.20	0.56
1:B:928:ASN:HB2	1:B:930:ILE:HD13	1.87	0.56
1:A:165:ILE:HD11	1:A:181:ILE:HB	1.85	0.56
1:B:402:ARG:NE	1:B:402:ARG:HA	2.19	0.56
1:B:401:GLY:C	1:B:403:GLY:H	2.07	0.56
1:B:983:ILE:N	1:B:983:ILE:HD12	2.18	0.56
1:A:165:ILE:HB	1:A:180:SER:OG	2.06	0.56
1:A:593:VAL:CG2	1:A:602:VAL:HG22	2.34	0.56
1:A:1019:ASN:H	1:A:1019:ASN:ND2	1.96	0.56
1:B:1020:LEU:H	1:B:1020:LEU:HD12	1.70	0.56
1:B:635:GLU:HB3	1:B:696:GLN:NE2	2.20	0.56
1:A:62:LYS:HG2	1:A:506:THR:HG23	1.88	0.56
1:A:81:ASP:O	1:A:85:LYS:HG3	2.06	0.56
1:A:857:TYR:CZ	1:A:860:ASP:HA	2.41	0.56
1:B:143:ILE:HG23	1:B:490:LEU:HD23	1.87	0.56
1:B:596:ILE:HG21	1:B:599:ILE:HD12	1.88	0.56
1:A:981:ASN:HA	1:A:1117:LEU:O	2.05	0.56
1:A:635:GLU:H	1:A:696:GLN:HE21	1.53	0.56
1:B:1131:ARG:HG2	1:B:1133:ASN:ND2	2.21	0.56
1:B:111:ASN:ND2	1:B:484:SER:HB2	2.21	0.56
1:A:13:VAL:HG13	1:A:19:LEU:HA	1.87	0.56
1:A:198:CYS:SG	1:A:759:ASP:OD2	2.64	0.56
1:B:42:ILE:HG22	1:B:44:GLU:HG2	1.86	0.56
1:B:454:ILE:HG21	1:B:666:ALA:HB2	1.88	0.56
1:B:82:ARG:HD3	1:B:82:ARG:O	2.06	0.56
1:B:898:VAL:HB	1:B:1031:PHE:HB2	1.88	0.56
1:A:453:GLU:HG2	1:A:454:ILE:HD13	1.88	0.56
1:A:578:GLN:O	1:A:578:GLN:HG3	2.04	0.56
1:A:722:LYS:C	1:A:724:ASN:H	2.07	0.56
1:A:833:ASP:CG	1:A:836:LEU:HD23	2.26	0.56
1:A:960:ILE:N	1:A:960:ILE:HD12	2.20	0.56
1:B:1096:ASN:HD22	1:B:1096:ASN:N	2.01	0.56
1:B:127:GLY:HA2	1:B:493:GLN:NE2	2.21	0.56
1:B:627:LEU:HD13	1:B:627:LEU:O	2.05	0.55
1:B:459:THR:O	1:B:459:THR:HG22	2.06	0.55
1:B:636:PHE:N	1:B:696:GLN:HE22	2.04	0.55
1:B:86:ILE:HD11	1:B:363:LEU:HB2	1.87	0.55
1:B:995:ILE:HD12	1:B:995:ILE:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:HZ3	1:A:478:GLU:C	2.09	0.55
1:B:116:ASN:ND2	1:B:118:ASN:H	2.01	0.55
1:B:299:TYR:HD1	1:B:302:VAL:HG11	1.72	0.55
1:B:191:SER:HB2	1:B:360:LEU:HD11	1.87	0.55
1:B:961:TRP:CE2	1:B:995:ILE:HG21	2.42	0.55
1:A:576:ILE:O	1:A:579:VAL:HG22	2.07	0.55
1:A:738:TYR:O	1:A:742:GLN:O	2.24	0.55
1:A:1168:THR:HG22	1:A:1169:THR:H	1.72	0.55
1:A:149:ILE:HB	1:A:183:ILE:HD13	1.87	0.55
1:B:1091:VAL:O	1:B:1094:PRO:HD3	2.06	0.55
1:B:252:PHE:CD2	1:B:262:ILE:HD12	2.42	0.55
1:B:203:ILE:HD11	1:B:396:ILE:HD11	1.88	0.55
1:B:571:LEU:HD12	1:B:571:LEU:N	2.22	0.55
1:A:523:LEU:HD11	1:A:703:GLN:HG2	1.89	0.55
1:A:857:TYR:OH	1:A:860:ASP:HA	2.07	0.55
1:B:939:ILE:HG21	1:B:1042:ILE:HD13	1.87	0.55
1:B:116:ASN:HD22	1:B:118:ASN:N	2.02	0.55
1:B:454:ILE:HG13	1:B:456:ASP:OD1	2.07	0.55
1:A:295:LEU:HD12	1:A:295:LEU:H	1.72	0.55
1:B:1071:ILE:O	1:B:1073:LYS:HE3	2.07	0.55
1:B:522:TYR:CD1	1:B:611:ASN:HB2	2.41	0.55
1:B:720:GLU:O	1:B:724:ASN:HB2	2.06	0.55
1:B:73:TYR:CE2	1:B:74:LEU:HG	2.41	0.55
1:B:1111:ILE:HD12	1:B:1111:ILE:C	2.27	0.55
1:B:121:ASP:HB3	1:B:285:LYS:HE2	1.88	0.55
1:B:370:ASN:HD21	1:B:377:ILE:CG2	2.20	0.55
1:B:8:ASN:HB2	1:B:11:ASP:OD2	2.07	0.55
1:A:154:GLU:HB2	1:A:155:PRO:HD2	1.88	0.54
1:A:651:LYS:HG2	1:A:653:PHE:H	1.72	0.54
1:B:354:GLN:HG2	1:B:432:GLY:CA	2.37	0.54
1:A:191:SER:HB2	1:A:360:LEU:HD11	1.89	0.54
1:B:487:LYS:HD2	1:B:487:LYS:C	2.28	0.54
1:B:728:LEU:HD23	1:B:728:LEU:C	2.28	0.54
1:B:973:LEU:HD23	1:B:1005:LEU:HB2	1.88	0.54
1:B:1131:ARG:HG2	1:B:1133:ASN:HD21	1.72	0.54
1:B:943:MET:HG3	1:B:950:TRP:O	2.07	0.54
1:A:988:ASN:HB2	5:A:1259:HOH:O	2.07	0.54
1:B:109:LYS:HE3	1:B:479:SER:CB	2.26	0.54
1:B:1171:LYS:HZ1	1:B:1224:TRP:HB2	1.72	0.54
1:B:667:ILE:HG23	1:B:793:LEU:HD22	1.90	0.54
1:A:199:MET:HG2	1:A:705:TYR:OH	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ASP:OD1	1:B:669:ASN:ND2	2.40	0.54
1:A:103:LEU:O	1:A:107:LEU:HD12	2.08	0.54
1:A:33:PHE:CD2	1:A:33:PHE:N	2.75	0.53
1:A:912:TYR:O	1:A:999:ARG:HG3	2.08	0.53
1:B:448:ILE:HD11	1:B:646:LEU:CG	2.37	0.53
1:B:559:PHE:CD1	1:B:582:ASP:HB3	2.43	0.53
1:A:1113:SER:OG	1:A:1120:ARG:HD2	2.07	0.53
1:A:271:ILE:O	1:A:275:LEU:HB2	2.08	0.53
1:A:362:ASN:ND2	1:A:364:LEU:H	2.05	0.53
1:A:907:ILE:CD1	1:A:1027:ASP:HA	2.38	0.53
1:A:1194:GLY:O	1:A:1196:ASN:N	2.40	0.53
1:A:81:ASP:OD2	1:A:85:LYS:HE3	2.07	0.53
1:A:920:TRP:HB2	1:A:1045:ARG:CG	2.38	0.53
1:A:295:LEU:HD12	1:A:295:LEU:N	2.24	0.53
1:A:723:TYR:CE2	1:A:731:LYS:HG3	2.44	0.53
1:B:409:ILE:N	1:B:409:ILE:HD12	2.23	0.53
1:B:973:LEU:CD2	1:B:1005:LEU:HB2	2.38	0.53
1:B:109:LYS:NZ	1:B:478:GLU:HB2	2.23	0.53
1:B:632:ILE:CG2	1:B:633:LEU:HD22	2.36	0.53
1:B:965:ASP:HB2	1:B:1020:LEU:HB3	1.89	0.53
1:A:1050:PHE:CD2	1:A:1054:LEU:HD11	2.44	0.53
1:A:93:ARG:HG3	1:A:371:ILE:O	2.08	0.53
1:A:448:ILE:CD1	1:A:643:PRO:HG2	2.35	0.53
1:A:877:ASP:O	1:A:896:SER:HB2	2.07	0.53
1:B:1215:LYS:O	1:B:1216:ALA:HB3	2.08	0.53
1:B:76:SER:O	1:B:80:LYS:HG3	2.09	0.53
1:A:148:VAL:HG22	1:A:182:ALA:HB3	1.89	0.53
1:A:279:TYR:HE2	1:A:327:ILE:HG21	1.74	0.53
1:A:289:VAL:HG13	1:A:289:VAL:O	2.09	0.53
1:A:299:TYR:HA	1:A:302:VAL:HG12	1.91	0.53
1:A:627:LEU:HD22	1:A:627:LEU:O	2.08	0.53
1:B:154:GLU:HB2	1:B:155:PRO:HD2	1.89	0.53
1:A:202:PHE:C	1:A:203:ILE:HD12	2.29	0.53
1:A:62:LYS:CG	1:A:506:THR:HG23	2.39	0.53
1:A:672:LYS:NZ	1:A:849:SER:OG	2.33	0.53
1:A:852:VAL:HG13	1:A:906:ILE:HG23	1.90	0.53
1:A:93:ARG:HG3	1:A:93:ARG:HH11	1.74	0.53
1:B:197:ASN:O	1:B:199:MET:N	2.41	0.53
1:B:370:ASN:HD21	1:B:377:ILE:HG22	1.73	0.53
1:B:378:ASN:H	1:B:378:ASN:HD22	1.56	0.53
1:B:454:ILE:HD12	1:B:666:ALA:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:LEU:HD12	1:B:836:LEU:N	2.24	0.53
1:A:166:SER:CB	1:A:498:ILE:HB	2.39	0.53
1:B:778:LYS:HA	1:B:782:LEU:HB2	1.90	0.53
1:B:910:ASN:O	1:B:912:TYR:N	2.39	0.53
1:B:121:ASP:OD2	1:B:121:ASP:N	2.41	0.52
1:B:203:ILE:N	1:B:203:ILE:HD12	2.24	0.52
1:B:999:ARG:HB3	1:B:999:ARG:NH1	2.24	0.52
1:B:1116:LEU:O	1:B:1117:LEU:HB2	2.09	0.52
1:B:1130:GLN:NE2	1:B:1151:ASN:ND2	2.49	0.52
1:B:727:THR:O	1:B:729:GLU:N	2.42	0.52
1:A:94:ILE:HG22	1:A:104:LEU:CD1	2.39	0.52
1:A:1190:MET:HE2	1:A:1199:MET:HG2	1.88	0.52
1:A:827:LEU:HD12	1:A:828:SER:N	2.24	0.52
1:B:36:MET:SD	1:B:104:LEU:HB3	2.50	0.52
1:B:199:MET:SD	1:B:199:MET:C	2.87	0.52
1:A:548:GLN:HA	5:A:1313:HOH:O	2.08	0.52
1:A:668:ASN:ND2	1:A:913:LYS:HZ1	2.06	0.52
1:A:924:PRO:O	1:A:1040:ARG:NH2	2.42	0.52
1:B:852:VAL:HG13	1:B:906:ILE:HG13	1.92	0.52
1:B:196:ASP:OD2	1:B:348:ARG:HA	2.10	0.52
1:B:270:ASP:O	1:B:274:ASN:HB2	2.10	0.52
1:A:555:PHE:CD1	1:A:586:GLU:HB3	2.44	0.52
1:A:888:PHE:CZ	1:A:1044:ILE:HG12	2.44	0.52
1:B:1200:ASN:HB2	1:B:1211:LEU:CD1	2.39	0.52
1:B:751:VAL:HG13	1:B:752:SER:N	2.24	0.52
1:B:912:TYR:O	1:B:999:ARG:HG3	2.10	0.52
1:B:1108:ILE:O	1:B:1108:ILE:HG13	2.10	0.52
1:B:429:ILE:HD13	1:B:429:ILE:N	2.24	0.52
1:B:973:LEU:HD21	1:B:1003:SER:O	2.09	0.52
1:B:800:HIS:O	1:B:803:ILE:HB	2.10	0.52
1:A:1214:PHE:HA	1:A:1220:VAL:HG22	1.92	0.52
1:A:106:GLU:HG2	1:A:330:LYS:HD2	1.90	0.52
1:A:556:SER:O	1:A:560:ILE:HG13	2.10	0.52
1:A:888:PHE:CZ	1:A:1044:ILE:CG1	2.93	0.52
1:B:994:THR:HG21	1:B:1059:ILE:HD12	1.91	0.52
1:B:154:GLU:HB2	1:B:155:PRO:CD	2.39	0.52
1:B:352:ILE:HD12	1:B:695:THR:HG22	1.91	0.52
1:B:944:ARG:HD3	1:B:945:ASP:H	1.73	0.52
1:A:287:SER:HB3	1:A:316:ILE:HA	1.92	0.52
1:B:297:ASN:N	1:B:298:PRO:CD	2.73	0.52
1:B:36:MET:CE	1:B:39:ILE:HD12	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:PHE:H	1:B:696:GLN:HE22	1.57	0.52
1:A:774:ILE:O	1:A:777:VAL:HG12	2.10	0.51
1:A:1006:TYR:CE2	1:A:1056:GLU:HG2	2.39	0.51
1:B:119:THR:HG21	1:B:125:HIS:CD2	2.45	0.51
1:B:913:LYS:HG3	1:B:914:ASN:CG	2.30	0.51
1:A:1038:TYR:OH	1:A:1040:ARG:NH1	2.43	0.51
1:B:110:ALA:HB1	1:B:221:LEU:HB3	1.92	0.51
1:B:693:ILE:HG21	1:B:769:TYR:CD2	2.46	0.51
1:B:868:TYR:HB3	1:B:903:ASN:OD1	2.09	0.51
1:B:1233:THR:O	1:B:1235:SER:N	2.43	0.51
1:A:68:TYR:CD2	1:A:157:LEU:HD22	2.45	0.51
1:B:910:ASN:C	1:B:912:TYR:H	2.13	0.51
1:A:476:ASN:HD21	1:A:1144:LYS:HB3	1.75	0.51
1:A:214:LEU:O	1:A:217:SER:HB2	2.11	0.51
1:A:712:VAL:HG13	1:A:747:LEU:HD13	1.91	0.51
1:B:1103:ASP:O	1:B:1104:SER:OG	2.25	0.51
1:B:1126:LYS:HB2	1:B:1153:VAL:CG2	2.40	0.51
1:B:267:GLN:O	1:B:271:ILE:HG13	2.11	0.51
1:B:728:LEU:HD23	1:B:728:LEU:O	2.10	0.51
1:B:777:VAL:HG13	1:B:778:LYS:N	2.26	0.51
1:A:1109:ASN:HB3	1:A:1217:ASP:CB	2.40	0.51
1:A:263:ILE:N	1:A:263:ILE:HD12	2.26	0.51
1:A:614:ASN:O	1:A:618:LYS:HG3	2.11	0.51
1:A:635:GLU:H	1:A:696:GLN:HE22	1.57	0.51
1:B:244:ILE:HG13	1:B:245:ARG:N	2.26	0.51
1:B:474:ASN:HD22	1:B:1070:ASN:HD22	1.59	0.51
1:B:593:VAL:CG2	1:B:602:VAL:HG23	2.40	0.51
1:B:924:PRO:HD2	1:B:1040:ARG:HH21	1.74	0.51
1:B:979:ASN:O	1:B:980:ALA:O	2.29	0.51
1:B:1139:ASP:OD2	1:B:1141:LEU:HG	2.10	0.51
1:B:378:ASN:N	1:B:378:ASN:ND2	2.59	0.51
1:B:541:ILE:HG23	1:B:542:ASP:N	2.26	0.51
1:B:660:LYS:HG2	1:B:804:LEU:CB	2.29	0.51
1:B:852:VAL:HG13	1:B:906:ILE:HG12	1.93	0.51
1:B:857:TYR:H	1:B:886:ASN:HD21	1.56	0.51
1:B:299:TYR:CA	1:B:302:VAL:HG12	2.40	0.51
1:B:670:ALA:CB	1:B:793:LEU:HD21	2.41	0.51
1:A:122:ASN:HA	1:A:288:LYS:O	2.10	0.50
1:A:1251:GLU:HG2	1:A:1251:GLU:O	2.11	0.50
1:B:606:ILE:HB	1:B:621:PHE:CE1	2.46	0.50
1:B:712:VAL:HG22	1:B:747:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:943:MET:HG2	1:B:948:SER:O	2.10	0.50
1:A:379:ASN:N	1:A:379:ASN:ND2	2.57	0.50
1:A:567:VAL:HG11	1:A:722:LYS:CA	2.41	0.50
1:B:116:ASN:C	1:B:116:ASN:HD22	2.14	0.50
1:B:856:ARG:HH21	1:B:1048:ASN:ND2	2.07	0.50
1:A:1166:THR:HG21	1:A:1209:ILE:HD12	1.92	0.50
1:A:370:ASN:ND2	1:A:377:ILE:HG21	2.26	0.50
1:A:454:ILE:HG21	1:A:666:ALA:CB	2.40	0.50
1:A:852:VAL:CG1	1:A:906:ILE:HD12	2.24	0.50
1:B:392:ASN:N	1:B:393:PRO:HD3	2.25	0.50
1:B:923:ILE:HD12	1:B:954:LEU:HD11	1.92	0.50
1:A:996:THR:CG2	1:A:1004:LYS:HB2	2.39	0.50
1:A:168:ARG:HG2	1:A:169:ASN:N	2.27	0.50
1:B:942:CYS:HB2	1:B:1029:ILE:HG23	1.94	0.50
1:B:474:ASN:ND2	1:B:1070:ASN:HB2	2.25	0.50
1:B:855:MET:HE1	1:B:898:VAL:HG11	1.94	0.50
1:A:497:TYR:CE1	1:A:499:PRO:HD2	2.47	0.50
1:A:920:TRP:HB2	1:A:1045:ARG:HG2	1.92	0.50
1:A:928:ASN:C	1:A:930:ILE:H	2.15	0.50
1:B:519:VAL:O	1:B:523:LEU:HG	2.10	0.50
1:B:541:ILE:O	1:B:544:ALA:HB3	2.11	0.50
1:A:1115:ILE:HG12	1:A:1115:ILE:O	2.10	0.50
1:A:416:VAL:HA	1:A:421:ILE:O	2.11	0.50
1:A:635:GLU:N	1:A:696:GLN:NE2	2.52	0.50
1:A:890:ILE:HG22	1:A:891:TYR:N	2.26	0.50
1:B:576:ILE:O	1:B:576:ILE:HD12	2.12	0.50
1:A:795:ASN:O	1:A:799:GLN:HG2	2.12	0.50
1:A:1190:MET:HE1	1:A:1199:MET:HG2	1.92	0.50
1:A:1193:VAL:O	1:A:1193:VAL:HG22	2.12	0.50
1:A:453:GLU:OE2	1:A:673:GLU:HB2	2.11	0.50
1:A:716:LYS:HG2	1:A:738:TYR:OH	2.11	0.50
1:B:1096:ASN:N	1:B:1096:ASN:ND2	2.58	0.49
1:B:981:ASN:HA	1:B:1117:LEU:O	2.12	0.49
1:B:1208:ASN:HB3	1:B:1226:TYR:OH	2.12	0.49
1:B:715:ILE:HA	1:B:718:ILE:HG22	1.94	0.49
1:A:111:ASN:HD21	1:A:484:SER:CB	2.24	0.49
1:A:1002:ASP:OD2	1:A:1002:ASP:N	2.44	0.49
1:A:323:LYS:O	1:A:327:ILE:HG12	2.12	0.49
1:B:1144:LYS:HE2	1:B:1192:SER:HB3	1.94	0.49
1:B:196:ASP:CG	1:B:348:ARG:HA	2.32	0.49
1:B:297:ASN:N	1:B:298:PRO:HD2	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:TRP:CE2	1:B:144:LEU:HD21	2.47	0.49
1:B:1150:ILE:HG12	1:B:1188:VAL:HG11	1.94	0.49
1:B:299:TYR:HA	1:B:302:VAL:CG1	2.41	0.49
1:B:525:ALA:HB2	1:B:545:LEU:CD2	2.43	0.49
1:B:924:PRO:O	1:B:1040:ARG:NH2	2.45	0.49
1:A:135:LYS:HA	1:A:140:SER:O	2.13	0.49
1:A:165:ILE:HD12	1:A:181:ILE:HB	1.93	0.49
1:A:876:GLY:HA3	1:A:895:LEU:O	2.11	0.49
1:A:961:TRP:CE2	1:A:995:ILE:HG21	2.48	0.49
1:B:926:TYR:O	1:B:1250:GLN:HB2	2.12	0.49
1:B:903:ASN:HD22	1:B:903:ASN:C	2.16	0.49
1:A:738:TYR:O	1:A:743:ILE:HB	2.11	0.49
1:B:1184:PHE:O	1:B:1186:GLN:HG3	2.12	0.49
1:B:719:ILE:CG2	1:B:738:TYR:HE1	2.25	0.49
1:A:593:VAL:HG21	1:A:625:LEU:HD23	1.95	0.49
1:A:832:ASP:O	1:A:833:ASP:HB2	2.13	0.49
1:A:454:ILE:HD13	1:A:454:ILE:N	2.28	0.49
1:B:295:LEU:CD1	1:B:295:LEU:H	2.17	0.49
1:B:575:TRP:O	1:B:579:VAL:HG13	2.12	0.49
1:B:943:MET:HA	1:B:948:SER:O	2.12	0.49
1:A:34:ASN:HB2	1:A:40:TRP:CH2	2.47	0.49
1:A:568:GLN:HB2	1:A:571:LEU:CD1	2.30	0.49
1:A:983:ILE:CD1	1:A:1094:PRO:HB3	2.43	0.49
1:A:394:ARG:HG2	1:A:394:ARG:HH11	1.77	0.49
1:A:417:SER:O	1:A:419:LYS:N	2.46	0.49
1:A:302:VAL:CG2	1:A:483:LEU:HD22	2.39	0.49
1:B:661:ASN:ND2	1:B:1000:LEU:HD21	2.27	0.49
1:B:920:TRP:O	1:B:1044:ILE:HA	2.12	0.49
1:B:160:THR:HG21	1:B:209:THR:HG22	1.95	0.49
1:B:21:ILE:HG12	1:B:134:ILE:CG2	2.42	0.49
1:B:233:ILE:HA	1:B:442:SER:OG	2.13	0.49
1:B:510:GLU:HG2	1:B:512:HIS:HE1	1.78	0.49
1:B:1114:THR:CG2	1:B:1117:LEU:H	2.25	0.48
1:B:576:ILE:O	1:B:579:VAL:HG22	2.12	0.48
1:A:704:MET:CG	1:A:758:ILE:HD13	2.42	0.48
1:B:1100:ARG:HH11	1:B:1100:ARG:HG2	1.79	0.48
1:B:409:ILE:O	1:B:429:ILE:HD13	2.14	0.48
1:B:800:HIS:HA	1:B:803:ILE:HD12	1.95	0.48
1:B:874:ILE:C	1:B:874:ILE:HD12	2.33	0.48
1:A:467:ASP:HB3	1:A:470:GLN:CB	2.41	0.48
1:B:856:ARG:NH2	1:B:1048:ASN:ND2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1189:VAL:CG2	1:B:1200:ASN:HB3	2.43	0.48
1:A:1072:LEU:HG	1:A:1192:SER:OG	2.14	0.48
1:A:129:ALA:HB2	1:A:167:LEU:HD11	1.94	0.48
1:A:106:GLU:OE2	1:A:477:SER:O	2.32	0.48
1:A:497:TYR:CD1	1:A:498:ILE:N	2.82	0.48
1:A:941:ASN:HD22	1:A:942:CYS:H	1.61	0.48
1:B:1064:SER:O	1:B:1069:THR:HG22	2.14	0.48
1:B:447:ASN:C	1:B:449:ASN:H	2.17	0.48
1:A:391:LEU:O	1:A:393:PRO:HD3	2.13	0.48
1:A:392:ASN:N	1:A:393:PRO:HD3	2.25	0.48
1:A:487:LYS:O	1:A:488:LEU:O	2.32	0.48
1:A:497:TYR:CD1	1:A:499:PRO:HD2	2.48	0.48
1:B:14:ASN:C	1:B:16:ARG:H	2.16	0.48
1:B:663:VAL:CG2	1:B:804:LEU:HD23	2.44	0.48
1:A:1006:TYR:O	1:A:1007:ILE:HD13	2.14	0.48
1:A:1033:ILE:HD11	1:A:1042:ILE:HG12	1.95	0.48
1:A:407:LYS:HD2	1:A:431:ASN:HB2	1.95	0.48
1:A:109:LYS:CG	1:A:483:LEU:HD21	2.43	0.48
1:A:686:VAL:O	1:A:690:MET:HG3	2.13	0.48
1:B:1251:GLU:CG	1:B:1252:LYS:H	2.21	0.48
1:B:299:TYR:O	1:B:302:VAL:HG12	2.13	0.48
1:B:320:ASN:HB3	1:B:323:LYS:HG2	1.94	0.48
1:B:610:LEU:HG	1:B:704:MET:HE1	1.94	0.48
1:B:681:VAL:O	1:B:685:ILE:HG12	2.13	0.48
1:B:798:ILE:HG13	1:B:799:GLN:N	2.27	0.48
1:A:415:ILE:HD12	1:A:425:ILE:HD12	1.96	0.48
1:A:733:GLU:O	1:A:734:LEU:HD23	2.13	0.48
1:A:854:ASN:HD22	1:A:866:SER:CA	2.26	0.48
1:B:249:ILE:HA	1:B:252:PHE:CD1	2.46	0.48
1:B:492:ILE:C	1:B:492:ILE:HD12	2.34	0.48
1:B:499:PRO:O	1:B:500:LYS:HB2	2.13	0.48
1:B:548:GLN:N	1:B:549:PRO:HD2	2.28	0.48
1:B:83:PHE:O	1:B:86:ILE:HG22	2.14	0.48
1:B:851:SER:OG	1:B:854:ASN:ND2	2.45	0.48
1:A:109:LYS:C	1:A:111:ASN:H	2.16	0.48
1:B:197:ASN:HD21	1:B:346:LYS:CD	2.17	0.48
1:B:916:SER:HB2	1:B:1054:LEU:HG	1.96	0.48
1:A:143:ILE:HG12	1:A:489:ASN:O	2.14	0.48
1:A:329:LYS:HZ3	1:A:466:ASN:HD21	1.62	0.48
1:A:925:ASN:O	1:A:927:ASP:N	2.46	0.48
1:B:305:ALA:HB1	1:B:479:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ILE:C	1:B:474:ASN:H	2.16	0.48
1:B:510:GLU:HG2	1:B:512:HIS:CE1	2.49	0.48
1:A:556:SER:HB2	1:A:558:GLU:HG2	1.96	0.48
1:B:359:LYS:O	1:B:397:THR:HG22	2.14	0.48
1:B:606:ILE:HG12	1:B:704:MET:CE	2.32	0.48
1:A:664:ILE:HD13	1:A:811:LEU:HD11	1.95	0.47
1:B:562:ASN:HD22	1:B:562:ASN:N	2.10	0.47
1:A:529:PRO:CG	1:A:532:GLU:HG3	2.44	0.47
1:A:81:ASP:CG	1:A:85:LYS:HE3	2.35	0.47
1:B:1114:THR:HG21	1:B:1117:LEU:N	2.29	0.47
1:A:146:PRO:O	1:A:181:ILE:HG12	2.14	0.47
1:A:252:PHE:CD2	1:A:262:ILE:HD12	2.49	0.47
1:A:21:ILE:O	1:A:29:PHE:HA	2.14	0.47
1:B:1252:LYS:CE	1:B:1252:LYS:HA	2.44	0.47
1:A:203:ILE:HD12	1:A:203:ILE:N	2.29	0.47
1:A:272:TYR:HA	1:A:328:PHE:CZ	2.48	0.47
1:A:467:ASP:O	1:A:470:GLN:HB3	2.13	0.47
1:A:111:ASN:HD21	1:A:484:SER:HB2	1.80	0.47
1:A:971:GLN:HA	1:A:971:GLN:NE2	2.29	0.47
1:B:1185:ASN:HA	1:B:1204:ASN:ND2	2.29	0.47
1:B:602:VAL:O	1:B:604:PRO:HD3	2.14	0.47
1:B:75:GLN:HA	1:B:75:GLN:HE21	1.80	0.47
1:A:854:ASN:ND2	1:A:866:SER:HA	2.28	0.47
1:A:868:TYR:CD2	1:A:906:ILE:HD11	2.49	0.47
1:B:1137:THR:CG2	1:B:1137:THR:O	2.51	0.47
1:B:369:TYR:HA	1:B:374:GLY:O	2.15	0.47
1:B:109:LYS:HZ2	1:B:478:GLU:HB2	1.79	0.47
1:B:928:ASN:C	1:B:930:ILE:N	2.68	0.47
1:A:852:VAL:CG1	1:A:906:ILE:HG23	2.43	0.47
1:B:1075:PHE:HD1	1:B:1241:ASN:HD22	1.62	0.47
1:B:516:GLU:HA	1:B:516:GLU:OE2	2.14	0.47
1:B:713:ASN:C	1:B:715:ILE:H	2.17	0.47
1:B:1126:LYS:HB2	1:B:1153:VAL:HG22	1.96	0.47
1:B:1193:VAL:CG2	1:B:1239:PHE:CE2	2.98	0.47
1:B:396:ILE:HG22	1:B:397:THR:H	1.79	0.47
1:B:412:CYS:O	1:B:514:VAL:HG22	2.15	0.47
1:A:529:PRO:HG2	1:A:532:GLU:CG	2.44	0.47
1:B:1066:GLU:N	1:B:1067:PRO:CD	2.78	0.47
1:B:306:LYS:HD3	1:B:307:TYR:CE1	2.49	0.47
1:B:484:SER:O	1:B:485:ASP:HB2	2.14	0.47
1:B:879:TYR:O	1:B:888:PHE:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:939:ILE:HG13	1:B:940:ILE:N	2.29	0.47
1:A:109:LYS:HZ3	1:A:479:SER:HB2	1.80	0.47
1:B:1114:THR:CG2	1:B:1117:LEU:N	2.78	0.47
1:B:211:MET:SD	1:B:339:LEU:HD22	2.54	0.47
1:B:971:GLN:NE2	1:B:1015:LYS:HB3	2.29	0.47
1:A:286:LEU:HD11	1:A:300:LYS:HA	1.97	0.47
1:A:89:LYS:HG3	1:A:371:ILE:HD11	1.97	0.47
1:A:548:GLN:N	1:A:549:PRO:HD2	2.29	0.47
1:B:1202:LYS:HB2	1:B:1207:ASN:O	2.15	0.47
1:B:122:ASN:HB3	1:B:288:LYS:HE2	1.97	0.47
1:B:497:TYR:HB3	1:B:498:ILE:H	1.41	0.47
1:B:620:ASN:ND2	1:B:620:ASN:N	2.63	0.47
1:B:701:LYS:CG	1:B:762:LEU:HD12	2.45	0.47
1:B:660:LYS:HE3	1:B:804:LEU:HB2	1.95	0.47
1:B:955:ASN:HB3	1:B:958:GLU:HG2	1.96	0.47
1:A:476:ASN:ND2	1:A:1144:LYS:HB3	2.30	0.46
1:A:584:THR:OG1	1:A:750:LYS:HE2	2.15	0.46
1:B:427:ILE:HD13	1:B:521:PHE:CD1	2.49	0.46
1:B:857:TYR:OH	1:B:860:ASP:HA	2.16	0.46
1:A:1168:THR:HG22	1:A:1170:ASN:H	1.80	0.46
1:A:368:ILE:C	1:A:368:ILE:HD13	2.36	0.46
1:A:923:ILE:HG22	1:A:1040:ARG:NH2	2.30	0.46
1:B:919:PHE:HE1	1:B:921:VAL:HB	1.81	0.46
1:A:1188:VAL:HA	1:A:1200:ASN:O	2.15	0.46
1:A:392:ASN:O	1:A:395:ILE:HG12	2.14	0.46
1:A:448:ILE:HG22	1:A:646:LEU:CD1	2.46	0.46
1:B:160:THR:HG21	1:B:209:THR:CG2	2.46	0.46
1:B:561:ASN:C	1:B:562:ASN:HD22	2.18	0.46
1:A:1002:ASP:CB	1:A:1016:SER:HA	2.45	0.46
1:A:111:ASN:ND2	1:A:483:LEU:HD13	2.28	0.46
1:A:128:ASP:CB	1:A:496:ALA:HB2	2.45	0.46
1:B:941:ASN:ND2	1:B:941:ASN:N	2.61	0.46
1:A:299:TYR:O	1:A:302:VAL:HG12	2.15	0.46
1:A:592:THR:O	1:A:622:LYS:HE3	2.15	0.46
1:A:664:ILE:CD1	1:A:811:LEU:HD11	2.46	0.46
1:B:1185:ASN:HA	1:B:1204:ASN:HD21	1.80	0.46
1:B:172:MET:HB2	1:B:175:ASN:ND2	2.30	0.46
1:B:677:LYS:HG2	1:B:785:TYR:CZ	2.51	0.46
1:B:999:ARG:HH11	1:B:999:ARG:CB	2.28	0.46
1:A:1114:THR:HG22	5:A:1272:HOH:O	2.15	0.46
1:A:1189:VAL:HG13	1:A:1200:ASN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:HG	1:B:317:TYR:CE2	2.50	0.46
1:B:965:ASP:OD1	1:B:967:ALA:HB3	2.15	0.46
1:A:108:SER:OG	1:A:109:LYS:HD3	2.15	0.46
1:B:20:TYR:HA	1:B:30:TYR:O	2.16	0.46
1:B:522:TYR:O	1:B:526:GLN:HG3	2.16	0.46
1:B:928:ASN:HB3	1:B:930:ILE:HD13	1.97	0.46
1:A:320:ASN:HB3	1:A:323:LYS:CG	2.45	0.46
1:A:413:LYS:HG3	1:A:414:ASN:N	2.31	0.46
1:A:593:VAL:HG11	1:A:596:ILE:HD12	1.98	0.46
1:B:1126:LYS:O	1:B:1153:VAL:HG13	2.16	0.46
1:A:797:ILE:HG21	1:A:812:ASN:HD21	1.80	0.46
1:B:323:LYS:O	1:B:326:ASP:HB2	2.15	0.46
1:B:32:SER:OG	1:B:42:ILE:HG12	2.15	0.46
1:B:925:ASN:O	1:B:927:ASP:N	2.49	0.46
1:A:1012:ILE:O	1:A:1012:ILE:HG13	2.16	0.46
1:A:128:ASP:O	1:A:165:ILE:HD13	2.16	0.46
1:B:1005:LEU:HD12	1:B:1012:ILE:HG22	1.98	0.46
1:B:1074:ASP:HB3	1:B:1076:TRP:H	1.81	0.46
1:B:1150:ILE:HG22	1:B:1162:LEU:HD12	1.97	0.46
1:B:581:VAL:O	1:B:581:VAL:HG12	2.16	0.46
1:A:1224:TRP:CH2	1:A:1235:SER:HB2	2.52	0.45
1:A:272:TYR:HA	1:A:328:PHE:HZ	1.81	0.45
1:A:197:ASN:HD21	1:A:346:LYS:NZ	2.14	0.45
1:B:382:VAL:HG23	1:B:382:VAL:O	2.15	0.45
1:B:453:GLU:HB2	1:B:649:THR:O	2.16	0.45
1:B:876:GLY:HA3	1:B:895:LEU:O	2.16	0.45
1:A:1157:THR:O	1:A:1157:THR:HG22	2.15	0.45
1:A:928:ASN:HB3	1:A:930:ILE:HG13	1.98	0.45
1:B:663:VAL:HG23	1:B:804:LEU:HD23	1.97	0.45
1:A:23:PRO:HD2	1:A:26:CYS:SG	2.56	0.45
1:A:320:ASN:HB3	1:A:323:LYS:HG2	1.98	0.45
1:A:448:ILE:N	1:A:448:ILE:HD13	2.31	0.45
1:A:584:THR:O	1:A:588:ASN:HB2	2.16	0.45
1:B:1082:TYR:HE1	1:B:1148:VAL:HG11	1.80	0.45
1:B:1193:VAL:HG21	1:B:1239:PHE:CE2	2.52	0.45
1:B:208:LEU:HA	1:B:211:MET:HE2	1.99	0.45
1:B:396:ILE:HG22	1:B:397:THR:N	2.31	0.45
1:B:537:LEU:HA	1:B:551:ILE:O	2.17	0.45
1:B:75:GLN:HA	1:B:75:GLN:NE2	2.31	0.45
1:A:1188:VAL:HG21	1:A:1199:MET:HB3	1.98	0.45
1:A:438:ALA:HB3	1:A:692:LYS:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:MET:HE1	1:A:913:LYS:HD3	1.97	0.45
1:A:941:ASN:ND2	1:A:942:CYS:N	2.62	0.45
1:B:327:ILE:HG22	1:B:331:LEU:HD22	1.98	0.45
1:B:884:ASN:HD22	1:B:886:ASN:H	1.63	0.45
1:B:939:ILE:HG13	1:B:940:ILE:H	1.81	0.45
1:A:1046:TYR:HB3	1:A:1066:GLU:OE1	2.17	0.45
1:A:1116:LEU:O	1:A:1117:LEU:HB2	2.15	0.45
1:B:897:GLU:CD	1:B:1032:LYS:HD2	2.37	0.45
1:B:1121:LEU:HD12	1:B:1249:TRP:CE2	2.52	0.45
1:B:642:ILE:HD11	1:B:685:ILE:CD1	2.41	0.45
1:A:174:SER:O	1:A:223:GLY:HA2	2.16	0.45
1:A:308:GLY:HA3	1:A:323:LYS:HB3	1.99	0.45
1:A:593:VAL:CG2	1:A:602:VAL:CG2	2.94	0.45
1:B:484:SER:O	1:B:485:ASP:CB	2.64	0.45
1:B:498:ILE:CG1	1:B:498:ILE:O	2.52	0.45
1:B:719:ILE:HG22	1:B:719:ILE:O	2.17	0.45
1:A:1166:THR:HA	1:A:1173:LYS:HD2	1.98	0.45
1:A:897:GLU:OE1	1:A:1032:LYS:HD3	2.17	0.45
1:A:293:ASN:HB3	1:A:295:LEU:HD13	1.99	0.45
1:A:729:GLU:O	1:A:730:GLU:HG3	2.16	0.45
1:B:244:ILE:CG1	1:B:245:ARG:N	2.79	0.45
1:B:986:TYR:HB3	1:B:991:ILE:HD11	1.98	0.45
1:A:164:ASN:ND2	1:A:220:GLY:HA3	2.31	0.45
1:A:528:VAL:HG13	1:A:528:VAL:O	2.16	0.45
1:A:802:SER:C	1:A:803:ILE:HD12	2.37	0.45
1:A:836:LEU:HD12	1:A:837:ILE:CD1	2.46	0.45
1:B:395:ILE:HG13	1:B:396:ILE:HG13	1.99	0.45
1:B:449:ASN:O	1:B:451:PRO:HD2	2.17	0.45
1:A:942:CYS:SG	1:A:1029:ILE:HG12	2.57	0.45
1:A:749:GLN:O	1:A:753:ILE:HG12	2.17	0.45
1:A:871:ASN:ND2	1:A:873:ASN:OD1	2.49	0.45
1:B:135:LYS:HG2	1:B:141:GLN:HA	1.98	0.45
1:B:541:ILE:HG23	1:B:542:ASP:H	1.81	0.45
1:B:568:GLN:HB3	1:B:569:ALA:H	1.61	0.45
1:B:567:VAL:HG11	1:B:572:PHE:HD1	1.82	0.45
1:B:105:GLU:O	1:B:108:SER:HB3	2.17	0.44
1:B:320:ASN:HB3	1:B:323:LYS:CG	2.47	0.44
1:A:306:LYS:O	1:A:327:ILE:HD12	2.17	0.44
1:A:872:ILE:HG12	1:A:900:ILE:HG12	1.99	0.44
1:B:1230:ARG:O	1:B:1231:ASP:CB	2.65	0.44
1:B:141:GLN:HB3	1:B:490:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:THR:O	1:B:339:LEU:HB2	2.17	0.44
1:B:548:GLN:N	1:B:549:PRO:CD	2.80	0.44
1:B:742:GLN:O	1:B:744:GLU:N	2.50	0.44
1:B:893:ASP:CG	1:B:894:LYS:HG3	2.38	0.44
1:A:888:PHE:CE2	1:A:1044:ILE:HG13	2.52	0.44
1:A:1086:TYR:CE1	1:A:1244:SER:HB3	2.52	0.44
1:B:913:LYS:CG	1:B:914:ASN:H	2.31	0.44
1:A:1168:THR:HG22	1:A:1169:THR:N	2.31	0.44
1:A:1230:ARG:O	1:A:1231:ASP:CB	2.65	0.44
1:B:1233:THR:C	1:B:1235:SER:N	2.69	0.44
1:B:62:LYS:HG3	1:B:506:THR:OG1	2.18	0.44
1:B:522:TYR:CE1	1:B:611:ASN:HB2	2.53	0.44
1:B:595:LYS:HE3	1:B:626:GLU:OE2	2.16	0.44
1:B:601:ILE:CG2	1:B:760:ARG:HG2	2.47	0.44
1:B:97:ASN:O	1:B:101:GLY:N	2.42	0.44
1:A:126:ILE:HD12	1:A:126:ILE:N	2.33	0.44
1:A:456:ASP:N	1:A:456:ASP:OD1	2.50	0.44
1:B:136:PHE:CE2	1:B:142:ASP:OD2	2.70	0.44
1:B:491:THR:HB	1:B:493:GLN:OE1	2.18	0.44
1:B:593:VAL:HB	1:B:599:ILE:O	2.17	0.44
1:B:593:VAL:HG22	1:B:602:VAL:CG2	2.47	0.44
1:B:613:GLY:HA3	1:B:617:GLN:HE21	1.83	0.44
1:B:352:ILE:HD12	1:B:695:THR:CG2	2.47	0.44
1:B:996:THR:CG2	1:B:996:THR:O	2.65	0.44
1:A:992:PHE:CD2	1:A:1063:TYR:HB2	2.53	0.44
1:A:1143:ARG:HD2	5:A:1279:HOH:O	2.17	0.44
1:B:966:ASN:HD22	1:B:1022:ASN:HD22	1.64	0.44
1:B:43:PRO:HB2	1:B:80:LYS:HB3	1.99	0.44
1:B:559:PHE:HD1	1:B:582:ASP:HB3	1.83	0.44
1:B:359:LYS:HB3	1:B:397:THR:O	2.18	0.44
1:A:425:ILE:HD11	1:A:546:LEU:HD23	1.99	0.44
1:A:722:LYS:C	1:A:724:ASN:N	2.71	0.44
1:B:1188:VAL:CG2	1:B:1199:MET:HB3	2.46	0.44
1:A:595:LYS:HB2	1:A:626:GLU:OE1	2.18	0.44
1:A:709:GLN:HG2	5:A:1257:HOH:O	2.17	0.44
1:A:841:ASN:OD1	1:A:846:ARG:N	2.51	0.44
1:A:894:LYS:C	1:A:895:LEU:HD12	2.37	0.44
1:B:887:GLN:HG2	1:B:1045:ARG:HD2	2.00	0.44
1:A:920:TRP:HA	1:A:991:ILE:O	2.18	0.43
1:A:914:ASN:HA	1:A:997:ASN:O	2.18	0.43
1:A:1087:TYR:HB2	1:A:1243:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ILE:HG22	1:A:646:LEU:HD12	2.00	0.43
1:A:329:LYS:NZ	1:A:466:ASN:ND2	2.66	0.43
1:B:454:ILE:HB	1:B:666:ALA:HA	2.00	0.43
1:B:526:GLN:O	1:B:710:ASN:HB3	2.18	0.43
1:B:855:MET:CE	1:B:898:VAL:HG11	2.49	0.43
1:A:290:GLN:O	1:A:291:VAL:CG2	2.67	0.43
1:A:81:ASP:OD1	1:A:85:LYS:HE3	2.18	0.43
1:B:890:ILE:O	1:B:1041:TYR:HA	2.17	0.43
1:B:1100:ARG:NH1	1:B:1101:ARG:O	2.51	0.43
1:B:1130:GLN:HG2	1:B:1149:TYR:HB2	2.00	0.43
1:B:1244:SER:O	1:B:1246:GLU:HG3	2.18	0.43
1:B:310:ASP:OD2	1:B:320:ASN:HB2	2.19	0.43
1:B:475:PHE:H	1:B:475:PHE:HD1	1.65	0.43
1:A:365:ASN:HB3	1:A:368:ILE:HG22	1.99	0.43
1:A:492:ILE:HD12	1:A:493:GLN:N	2.32	0.43
1:A:737:LYS:HG2	1:A:741:LYS:HE3	1.99	0.43
1:A:8:ASN:HB2	1:A:11:ASP:OD2	2.18	0.43
1:A:9:TYR:HB2	1:A:81:ASP:HA	2.00	0.43
1:B:197:ASN:O	1:B:198:CYS:C	2.56	0.43
1:B:711:GLN:O	1:B:715:ILE:HG12	2.17	0.43
1:B:923:ILE:HD12	1:B:954:LEU:CD1	2.48	0.43
1:A:253:LEU:HA	1:A:253:LEU:HD12	1.84	0.43
1:B:145:LEU:N	1:B:145:LEU:HD12	2.33	0.43
1:B:302:VAL:HG13	1:B:303:PHE:N	2.32	0.43
1:B:444:ASN:ND2	1:B:446:ASP:OD1	2.52	0.43
1:B:670:ALA:HB1	1:B:793:LEU:HD21	1.99	0.43
1:B:846:ARG:O	1:B:847:ILE:O	2.36	0.43
1:A:1122:TYR:CE1	1:A:1245:GLU:HA	2.54	0.43
1:A:21:ILE:HG12	1:A:134:ILE:HG22	2.00	0.43
1:A:144:LEU:O	1:A:146:PRO:HD3	2.18	0.43
1:A:306:LYS:HD3	1:A:307:TYR:CE1	2.53	0.43
1:A:438:ALA:HB2	1:A:691:THR:HB	2.00	0.43
1:A:571:LEU:H	1:A:571:LEU:HD12	1.83	0.43
1:B:286:LEU:HD12	1:B:289:VAL:HG21	2.00	0.43
1:A:197:ASN:HD21	1:A:346:LYS:CE	2.32	0.43
1:A:738:TYR:CA	1:A:743:ILE:HD13	2.48	0.43
1:B:193:ARG:NH1	1:B:358:PHE:HZ	2.17	0.43
1:B:551:ILE:N	1:B:551:ILE:HD12	2.34	0.43
1:B:769:TYR:O	1:B:772:LYS:HB3	2.18	0.43
1:A:186:PHE:CE2	1:A:188:PRO:HB3	2.53	0.43
1:A:311:LYS:HB2	1:A:317:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLU:C	1:A:454:ILE:HG12	2.38	0.43
1:A:565:LYS:HB2	1:A:566:PRO:HD2	2.00	0.43
1:A:661:ASN:HD22	1:A:661:ASN:HA	1.69	0.43
1:A:742:GLN:C	1:A:743:ILE:HD12	2.39	0.43
1:A:797:ILE:HG21	1:A:812:ASN:ND2	2.33	0.43
1:A:830:TYR:O	1:A:831:THR:HG22	2.19	0.43
1:A:971:GLN:CA	1:A:971:GLN:HE21	2.31	0.43
1:B:409:ILE:HD13	1:B:431:ASN:HA	2.00	0.43
1:B:527:LYS:HB2	1:B:527:LYS:HE3	1.81	0.43
1:B:983:ILE:CG1	1:B:1094:PRO:HB2	2.48	0.43
1:A:121:ASP:HB2	1:A:288:LYS:HE2	2.01	0.43
1:A:214:LEU:CA	1:A:217:SER:HB2	2.48	0.43
1:A:304:GLU:OE1	1:A:317:TYR:HE1	2.02	0.43
1:A:82:ARG:NH2	1:A:362:ASN:ND2	2.67	0.43
1:A:234:THR:HG22	1:A:439:SER:HB3	2.01	0.43
1:A:920:TRP:O	1:A:1044:ILE:HA	2.18	0.43
1:B:536:ASN:O	1:B:537:LEU:HD12	2.17	0.43
1:B:983:ILE:HG12	1:B:1094:PRO:HB2	2.00	0.43
1:A:1114:THR:OG1	1:A:1117:LEU:N	2.52	0.43
1:A:376:ASN:ND2	1:A:386:GLY:CA	2.81	0.43
1:B:114:LEU:HD11	1:B:299:TYR:CD2	2.54	0.43
1:B:653:PHE:CE2	1:B:662:LYS:HB3	2.53	0.43
1:A:324:PHE:HA	1:A:327:ILE:HG12	1.99	0.42
1:A:772:LYS:O	1:A:776:GLU:HB2	2.18	0.42
1:B:1020:LEU:N	1:B:1020:LEU:HD12	2.34	0.42
1:B:1143:ARG:HG3	1:B:1143:ARG:HH11	1.84	0.42
1:B:528:VAL:HG13	1:B:528:VAL:O	2.19	0.42
1:B:727:THR:O	1:B:730:GLU:N	2.47	0.42
1:A:263:ILE:O	1:A:846:ARG:NH2	2.51	0.42
1:A:2:PRO:O	1:A:95:ASN:ND2	2.52	0.42
1:A:344:GLN:O	1:A:384:PHE:HE1	2.02	0.42
1:A:486:GLU:HB3	1:A:488:LEU:CD2	2.48	0.42
1:A:733:GLU:C	1:A:734:LEU:HD23	2.40	0.42
1:A:845:LYS:HZ2	1:A:848:LYS:HB3	1.83	0.42
1:A:971:GLN:HA	1:A:971:GLN:HE21	1.84	0.42
1:B:1004:LYS:HG2	1:B:1014:GLN:HB3	2.00	0.42
1:B:476:ASN:HD21	1:B:480:ALA:HB2	1.84	0.42
1:B:5:ASN:ND2	1:B:5:ASN:N	2.67	0.42
1:B:760:ARG:CZ	1:B:830:TYR:HD2	2.33	0.42
1:B:836:LEU:C	1:B:838:SER:H	2.23	0.42
1:B:884:ASN:C	1:B:884:ASN:ND2	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:916:SER:CB	1:B:1054:LEU:HG	2.50	0.42
1:A:116:ASN:C	1:A:118:ASN:H	2.22	0.42
1:A:295:LEU:O	1:A:298:PRO:HD2	2.19	0.42
1:A:557:SER:HA	1:A:560:ILE:HD12	2.01	0.42
1:A:909:ASP:O	1:A:910:ASN:O	2.37	0.42
1:B:1157:THR:HG22	1:B:1158:HIS:N	2.34	0.42
1:B:1193:VAL:CG2	1:B:1239:PHE:HE2	2.32	0.42
1:B:797:ILE:HG21	1:B:812:ASN:HD21	1.84	0.42
1:B:82:ARG:HH12	1:B:189:GLU:HG2	1.83	0.42
1:A:1099:ASP:OD1	1:A:1100:ARG:N	2.52	0.42
1:A:270:ASP:O	1:A:274:ASN:HB2	2.18	0.42
1:A:316:ILE:C	1:A:316:ILE:HD12	2.40	0.42
1:A:234:THR:HG22	1:A:439:SER:CB	2.50	0.42
1:A:937:TYR:HB2	1:A:1034:VAL:O	2.19	0.42
1:B:1087:TYR:HB2	1:B:1243:ILE:HB	2.01	0.42
1:B:324:PHE:C	1:B:326:ASP:N	2.73	0.42
1:B:606:ILE:HG23	1:B:704:MET:CE	2.50	0.42
1:B:855:MET:O	1:B:856:ARG:HD3	2.19	0.42
1:A:144:LEU:C	1:A:146:PRO:HD3	2.40	0.42
1:A:68:TYR:HD2	1:A:157:LEU:HD22	1.83	0.42
1:A:164:ASN:HB3	1:A:180:SER:HB3	2.02	0.42
1:A:452:LYS:HG3	1:A:452:LYS:H	1.65	0.42
1:A:672:LYS:HA	1:A:672:LYS:HD2	1.62	0.42
1:A:436:PHE:CD2	1:A:695:THR:HG21	2.55	0.42
1:A:76:SER:OG	1:A:79:GLU:HG3	2.18	0.42
1:A:910:ASN:HA	1:A:1022:ASN:OD1	2.19	0.42
1:B:111:ASN:HA	1:B:112:PRO:HD3	1.89	0.42
1:B:116:ASN:ND2	1:B:118:ASN:N	2.65	0.42
1:B:129:ALA:HB2	1:B:167:LEU:HD21	2.01	0.42
1:B:678:TRP:CE3	1:B:782:LEU:HD13	2.55	0.42
1:B:76:SER:HB3	1:B:79:GLU:OE2	2.19	0.42
1:B:941:ASN:HD22	1:B:941:ASN:H	1.67	0.42
1:A:595:LYS:CB	1:A:626:GLU:HB2	2.48	0.42
1:A:708:LEU:HD23	1:A:708:LEU:HA	1.83	0.42
1:A:45:ARG:HD3	1:A:74:LEU:HB2	2.00	0.42
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.88	0.42
1:A:944:ARG:HD3	1:A:944:ARG:HA	1.70	0.42
1:B:413:LYS:HE3	1:B:515:ASN:O	2.20	0.42
1:B:615:GLU:N	1:B:615:GLU:CD	2.72	0.42
1:A:379:ASN:H	1:A:379:ASN:ND2	2.09	0.42
1:A:632:ILE:HG23	1:A:633:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1189:VAL:HG22	1:B:1200:ASN:HB3	2.01	0.42
1:B:401:GLY:C	1:B:403:GLY:N	2.73	0.42
1:B:598:ASP:OD1	1:B:768:SER:HA	2.19	0.42
1:A:234:THR:HG22	1:A:439:SER:OG	2.18	0.42
1:A:541:ILE:HG23	1:A:542:ASP:N	2.35	0.42
1:A:737:LYS:HG2	1:A:741:LYS:HG2	2.02	0.42
1:B:1132:VAL:HG23	1:B:1148:VAL:CA	2.49	0.42
1:B:154:GLU:CB	1:B:155:PRO:CD	2.98	0.42
1:B:532:GLU:OE1	1:B:532:GLU:HA	2.20	0.42
1:B:771:MET:CE	1:B:825:PHE:HE2	2.33	0.42
1:A:321:ILE:HD13	1:A:321:ILE:HA	1.84	0.42
1:A:567:VAL:HB	1:A:726:TYR:OH	2.19	0.42
1:B:661:ASN:HA	1:B:661:ASN:HD22	1.65	0.42
1:B:999:ARG:NH1	1:B:999:ARG:CB	2.82	0.42
1:A:1065:ASN:HD22	1:A:1065:ASN:N	2.17	0.42
1:A:837:ILE:HB	1:A:838:SER:H	1.76	0.42
1:A:847:ILE:N	1:A:847:ILE:CD1	2.81	0.42
1:B:1228:HIS:HB3	1:B:1233:THR:OG1	2.20	0.42
1:B:1076:TRP:CZ3	1:B:1244:SER:O	2.72	0.42
1:B:111:ASN:ND2	1:B:483:LEU:HD12	2.29	0.42
1:B:743:ILE:C	1:B:745:ASN:H	2.22	0.42
1:A:14:ASN:ND2	1:A:16:ARG:NH1	2.68	0.41
1:A:270:ASP:HA	1:A:273:THR:CG2	2.50	0.41
1:A:453:GLU:CG	1:A:454:ILE:HD13	2.49	0.41
1:A:944:ARG:O	1:A:946:ASN:N	2.53	0.41
1:B:172:MET:CE	1:B:175:ASN:HD21	2.33	0.41
1:B:476:ASN:OD1	1:B:480:ALA:HB2	2.20	0.41
1:B:657:SER:O	1:B:658:ASP:HB3	2.21	0.41
1:B:836:LEU:CD1	1:B:836:LEU:N	2.83	0.41
1:B:93:ARG:HG3	1:B:93:ARG:NH1	2.25	0.41
1:A:975:PHE:CE2	1:A:1007:ILE:HG21	2.56	0.41
1:A:141:GLN:HE21	1:A:490:LEU:CD2	2.30	0.41
1:A:29:PHE:CD2	1:A:135:LYS:HE2	2.55	0.41
1:A:377:ILE:O	1:A:378:ASN:HB2	2.20	0.41
1:B:1136:SER:O	1:B:1137:THR:HB	2.20	0.41
1:B:35:ILE:HG23	1:B:36:MET:N	2.35	0.41
1:B:453:GLU:HG2	1:B:650:ILE:HG12	2.02	0.41
1:B:639:GLU:O	1:B:640:LEU:HD23	2.21	0.41
1:B:720:GLU:HG2	1:B:738:TYR:OH	2.20	0.41
1:B:842:LYS:HE3	1:B:843:PHE:CZ	2.55	0.41
1:B:893:ASP:OD2	1:B:894:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:PHE:HZ	1:B:150:ILE:HD11	1.85	0.41
1:A:193:ARG:HH11	1:A:193:ARG:CG	2.33	0.41
1:A:72:ASN:O	1:A:75:GLN:HG2	2.20	0.41
1:A:790:LYS:HB2	1:A:819:LEU:HD23	2.02	0.41
1:B:154:GLU:O	1:B:155:PRO:C	2.58	0.41
1:B:107:LEU:HD11	1:B:214:LEU:HB3	2.01	0.41
1:B:286:LEU:HA	1:B:289:VAL:HG23	2.02	0.41
1:B:208:LEU:HG	1:B:336:GLU:HG3	2.03	0.41
1:B:383:ASN:ND2	1:B:383:ASN:N	2.69	0.41
1:B:730:GLU:O	1:B:733:GLU:HG2	2.20	0.41
1:B:830:TYR:O	1:B:832:ASP:N	2.54	0.41
1:A:275:LEU:HB3	1:A:324:PHE:HZ	1.84	0.41
1:A:591:SER:O	1:A:601:ILE:HA	2.21	0.41
1:A:924:PRO:HB3	1:A:988:ASN:OD1	2.21	0.41
1:B:1166:THR:HG22	1:B:1209:ILE:HD12	2.03	0.41
1:B:320:ASN:OD1	1:B:322:ASN:HB2	2.19	0.41
1:B:586:GLU:C	1:B:588:ASN:H	2.23	0.41
1:B:853:LEU:HD12	1:B:854:ASN:H	1.86	0.41
1:A:57:PRO:HA	1:A:58:PRO:HD2	1.93	0.41
1:B:1067:PRO:O	1:B:1073:LYS:HE2	2.21	0.41
1:B:200:ASN:ND2	1:B:388:ASN:ND2	2.69	0.41
1:B:362:ASN:HD22	1:B:365:ASN:HB2	1.84	0.41
1:B:413:LYS:HG2	1:B:517:LEU:CD2	2.50	0.41
1:B:557:SER:HA	1:B:560:ILE:HD12	2.01	0.41
1:B:558:GLU:CD	1:B:558:GLU:H	2.22	0.41
1:B:788:ASN:HA	1:B:788:ASN:HD22	1.66	0.41
1:A:1200:ASN:ND2	1:A:1202:LYS:HD2	2.35	0.41
1:A:34:ASN:HB2	1:A:40:TRP:CZ2	2.56	0.41
1:A:454:ILE:HD12	1:A:669:ASN:HB2	2.03	0.41
1:A:915:PHE:O	1:A:997:ASN:HB2	2.20	0.41
1:B:110:ALA:O	1:B:111:ASN:C	2.58	0.41
1:B:370:ASN:ND2	1:B:377:ILE:CG2	2.83	0.41
1:B:701:LYS:HG3	1:B:762:LEU:HD12	2.02	0.41
1:A:11:ASP:HA	1:A:12:PRO:HD3	1.84	0.41
1:A:440:GLU:OE1	1:A:440:GLU:HA	2.20	0.41
1:B:61:LEU:HD13	1:B:405:VAL:CG1	2.51	0.41
1:A:1108:ILE:HG22	1:A:1217:ASP:HA	2.02	0.41
1:A:578:GLN:O	1:A:582:ASP:HB2	2.21	0.41
1:B:1090:ASN:HB2	1:B:1240:TRP:CZ3	2.56	0.41
1:B:453:GLU:CA	1:B:453:GLU:OE1	2.57	0.41
1:B:562:ASN:ND2	1:B:562:ASN:N	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:944:ARG:O	1:B:945:ASP:C	2.58	0.41
1:A:1058:GLU:HA	1:A:1061:THR:CG2	2.51	0.41
1:A:19:LEU:HD12	1:A:19:LEU:C	2.41	0.41
1:A:344:GLN:O	1:A:344:GLN:HG2	2.21	0.41
1:A:193:ARG:O	1:A:355:TYR:HB3	2.21	0.41
1:A:712:VAL:HG22	1:A:747:LEU:HB3	2.02	0.41
1:B:285:LYS:HZ2	1:B:285:LYS:HB3	1.85	0.41
1:B:425:ILE:CD1	1:B:545:LEU:HD13	2.51	0.41
1:B:606:ILE:HA	1:B:704:MET:HE3	2.02	0.41
1:B:999:ARG:NH2	1:B:1023:ILE:HD11	2.36	0.41
1:A:1163:TYR:CD2	1:A:1178:SER:HB2	2.56	0.40
1:A:193:ARG:HH11	1:A:193:ARG:HB3	1.86	0.40
1:A:348:ARG:HG2	5:A:1274:HOH:O	2.21	0.40
1:A:737:LYS:CB	1:A:741:LYS:HG2	2.50	0.40
1:B:1050:PHE:CE2	1:B:1054:LEU:HD11	2.56	0.40
1:B:203:ILE:HD11	1:B:389:ALA:HA	2.04	0.40
1:B:297:ASN:C	1:B:299:TYR:H	2.24	0.40
1:B:59:THR:HB	1:B:507:SER:HA	2.02	0.40
1:B:716:LYS:HB2	1:B:744:GLU:OE2	2.20	0.40
1:B:994:THR:HB	1:B:1006:TYR:HB2	2.03	0.40
1:A:1000:LEU:HA	1:A:1000:LEU:HD12	1.87	0.40
1:A:1071:ILE:HD13	1:A:1141:LEU:HD13	2.03	0.40
1:A:342:LYS:HA	1:A:342:LYS:CE	2.49	0.40
1:A:448:ILE:HG22	1:A:646:LEU:CB	2.51	0.40
1:A:143:ILE:O	1:A:487:LYS:O	2.39	0.40
1:B:1034:VAL:O	1:B:1035:ASN:HB2	2.21	0.40
1:B:157:LEU:HD23	1:B:190:TYR:CE1	2.55	0.40
1:B:700:ARG:HD3	1:B:703:GLN:HE22	1.86	0.40
1:A:453:GLU:HG2	1:A:454:ILE:CD1	2.51	0.40
1:A:410:ARG:CB	1:A:511:GLN:HG3	2.46	0.40
1:A:827:LEU:HD12	1:A:828:SER:H	1.85	0.40
1:B:1150:ILE:O	1:B:1162:LEU:HB2	2.20	0.40
1:B:149:ILE:HB	1:B:183:ILE:HD13	2.03	0.40
1:B:409:ILE:CD1	1:B:431:ASN:HA	2.51	0.40
1:B:535:VAL:HG11	1:B:717:THR:HG21	2.04	0.40
1:B:884:ASN:ND2	1:B:886:ASN:H	2.19	0.40
1:A:671:LEU:HD23	1:A:671:LEU:HA	1.88	0.40
1:A:737:LYS:O	1:A:739:ASP:N	2.54	0.40
1:A:819:LEU:HD12	1:A:819:LEU:HA	1.93	0.40
1:A:93:ARG:HG3	1:A:93:ARG:NH1	2.36	0.40
1:B:346:LYS:HA	1:B:346:LYS:CE	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:ASN:CB	1:B:1022:ASN:ND2	2.84	0.40
1:A:97:ASN:O	1:A:101:GLY:N	2.51	0.40
1:B:635:GLU:H	1:B:696:GLN:NE2	2.19	0.40
1:B:715:ILE:O	1:B:718:ILE:N	2.54	0.40
1:B:741:LYS:O	1:B:742:GLN:HG3	2.22	0.40
1:B:750:LYS:O	1:B:753:ILE:HB	2.21	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	1242/1252 (99%)	1056 (85%)	128 (10%)	58 (5%)	2	2
1	B	1232/1252 (98%)	1003 (81%)	171 (14%)	58 (5%)	2	2
All	All	2474/2504 (99%)	2059 (83%)	299 (12%)	116 (5%)	2	2

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ALA
1	A	198	CYS
1	A	290	GLN
1	A	418	VAL
1	A	419	LYS
1	A	485	ASP
1	A	488	LEU
1	A	489	ASN
1	A	740	ILE
1	A	805	GLY
1	A	834	LYS
1	A	837	ILE

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Mol	Chain	Res	Type
1	A	847	ILE
1	A	848	LYS
1	A	849	SER
1	A	910	ASN
1	A	914	ASN
1	A	927	ASP
1	A	928	ASN
1	A	945	ASP
1	A	980	ALA
1	A	1193	VAL
1	A	1195	ASN
1	A	1250	GLN
1	B	136	PHE
1	B	153	ALA
1	B	297	ASN
1	B	467	ASP
1	B	479	SER
1	B	485	ASP
1	B	497	TYR
1	B	728	LEU
1	B	743	ILE
1	B	831	THR
1	B	837	ILE
1	B	838	SER
1	B	847	ILE
1	B	848	LYS
1	B	849	SER
1	B	913	LYS
1	B	914	ASN
1	B	945	ASP
1	B	980	ALA
1	B	1144	LYS
1	B	1195	ASN
1	A	137	SER
1	A	297	ASN
1	A	417	SER
1	A	456	ASP
1	A	569	ALA
1	A	658	ASP
1	A	738	TYR
1	A	1062	LEU
1	A	1068	ASN

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Mol	Chain	Res	Type
1	A	1144	LYS
1	A	1231	ASP
1	A	1232	HIS
1	B	198	CYS
1	B	394	ARG
1	B	448	ILE
1	B	454	ILE
1	B	455	ASP
1	B	473	LEU
1	B	490	LEU
1	B	739	ASP
1	B	911	LYS
1	B	927	ASP
1	B	1016	SER
1	B	1231	ASP
1	B	1234	ASN
1	A	110	ALA
1	A	451	PRO
1	A	479	SER
1	A	723	TYR
1	A	730	GLU
1	A	839	TYR
1	B	98	LEU
1	B	486	GLU
1	B	656	SER
1	B	850	SER
1	B	884	ASN
1	B	1216	ALA
1	A	177	GLY
1	A	362	ASN
1	A	454	ILE
1	A	483	LEU
1	A	743	ILE
1	A	884	ASN
1	A	1194	GLY
1	B	15	ASP
1	B	110	ALA
1	B	366	ASP
1	B	453	GLU
1	B	483	LEU
1	B	725	SER
1	B	910	ASN

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Mol	Chain	Res	Type
1	B	1056	GLU
1	A	122	ASN
1	A	497	TYR
1	A	736	ASN
1	A	894	LYS
1	A	1021	GLY
1	A	1056	GLU
1	B	496	ALA
1	B	563	VAL
1	B	803	ILE
1	B	941	ASN
1	B	1068	ASN
1	A	118	ASN
1	A	737	LYS
1	B	658	ASP
1	B	1205	ASN
1	B	968	GLY
1	A	154	GLU
1	B	480	ALA
1	B	481	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	1146/1153 (99%)	1050 (92%)	96 (8%)	12	18
1	B	1139/1153 (99%)	1051 (92%)	88 (8%)	14	23
All	All	2285/2306 (99%)	2101 (92%)	184 (8%)	13	20

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	33	PHE
1	A	37	LYS

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Mol	Chain	Res	Type
1	A	61	LEU
1	A	65	ASP
1	A	78	GLU
1	A	98	LEU
1	A	107	LEU
1	A	109	LYS
1	A	118	ASN
1	A	166	SER
1	A	193	ARG
1	A	199	MET
1	A	217	SER
1	A	232	THR
1	A	234	THR
1	A	273	THR
1	A	275	LEU
1	A	328	PHE
1	A	331	LEU
1	A	347	CYS
1	A	348	ARG
1	A	368	ILE
1	A	379	ASN
1	A	433	GLU
1	A	445	ASP
1	A	448	ILE
1	A	452	LYS
1	A	453	GLU
1	A	456	ASP
1	A	467	ASP
1	A	486	GLU
1	A	488	LEU
1	A	494	ASN
1	A	538	THR
1	A	550	LYS
1	A	558	GLU
1	A	568	GLN
1	A	578	GLN
1	A	580	LEU
1	A	594	ASP
1	A	602	VAL
1	A	627	LEU
1	A	633	LEU
1	A	639	GLU

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Mol	Chain	Res	Type
1	A	661	ASN
1	A	675	ASP
1	A	676	GLU
1	A	677	LYS
1	A	735	THR
1	A	737	LYS
1	A	759	ASP
1	A	760	ARG
1	A	794	LEU
1	A	809	GLN
1	A	819	LEU
1	A	836	LEU
1	A	837	ILE
1	A	839	TYR
1	A	845	LYS
1	A	852	VAL
1	A	861	LYS
1	A	895	LEU
1	A	911	LYS
1	A	912	TYR
1	A	914	ASN
1	A	925	ASN
1	A	938	THR
1	A	941	ASN
1	A	947	ASN
1	A	962	THR
1	A	973	LEU
1	A	996	THR
1	A	1000	LEU
1	A	1005	LEU
1	A	1019	ASN
1	A	1024	HIS
1	A	1030	LEU
1	A	1039	THR
1	A	1044	ILE
1	A	1053	GLU
1	A	1055	ASP
1	A	1061	THR
1	A	1114	THR
1	A	1115	ILE
1	A	1128	LYS
1	A	1138	ASN

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Mol	Chain	Res	Type
1	A	1153	VAL
1	A	1185	ASN
1	A	1189	VAL
1	A	1211	LEU
1	A	1218	THR
1	A	1229	MET
1	A	1230	ARG
1	A	1232	HIS
1	A	1234	ASN
1	B	14	ASN
1	B	37	LYS
1	B	53	GLN
1	B	98	LEU
1	B	99	SER
1	B	111	ASN
1	B	116	ASN
1	B	133	GLU
1	B	155	PRO
1	B	186	PHE
1	B	199	MET
1	B	232	THR
1	B	234	THR
1	B	244	ILE
1	B	270	ASP
1	B	296	LEU
1	B	322	ASN
1	B	326	ASP
1	B	328	PHE
1	B	331	LEU
1	B	339	LEU
1	B	341	THR
1	B	346	LYS
1	B	349	GLN
1	B	399	ILE
1	B	402	ARG
1	B	423	LYS
1	B	429	ILE
1	B	442	SER
1	B	445	ASP
1	B	450	THR
1	B	452	LYS
1	B	453	GLU

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Mol	Chain	Res	Type
1	B	455	ASP
1	B	466	ASN
1	B	478	GLU
1	B	483	LEU
1	B	487	LYS
1	B	493	GLN
1	B	500	LYS
1	B	503	SER
1	B	506	THR
1	B	508	ASP
1	B	530	GLU
1	B	547	GLU
1	B	558	GLU
1	B	568	GLN
1	B	582	ASP
1	B	595	LYS
1	B	676	GLU
1	B	723	TYR
1	B	736	ASN
1	B	737	LYS
1	B	804	LEU
1	B	809	GLN
1	B	837	ILE
1	B	838	SER
1	B	840	PHE
1	B	860	ASP
1	B	884	ASN
1	B	903	ASN
1	B	906	ILE
1	B	911	LYS
1	B	912	TYR
1	B	913	LYS
1	B	914	ASN
1	B	927	ASP
1	B	941	ASN
1	B	944	ARG
1	B	945	ASP
1	B	965	ASP
1	B	983	ILE
1	B	996	THR
1	B	1044	ILE
1	B	1099	ASP

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Mol	Chain	Res	Type
1	B	1113	SER
1	B	1116	LEU
1	B	1131	ARG
1	B	1133	ASN
1	B	1138	ASN
1	B	1144	LYS
1	B	1153	VAL
1	B	1168	THR
1	B	1170	ASN
1	B	1195	ASN
1	B	1229	MET
1	B	1233	THR
1	B	1252	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	34	ASN
1	A	53	GLN
1	A	63	ASN
1	A	72	ASN
1	A	111	ASN
1	A	116	ASN
1	A	118	ASN
1	A	141	GLN
1	A	169	ASN
1	A	176	HIS
1	A	197	ASN
1	A	344	GLN
1	A	362	ASN
1	A	376	ASN
1	A	378	ASN
1	A	379	ASN
1	A	383	ASN
1	A	466	ASN
1	A	470	GLN
1	A	493	GLN
1	A	494	ASN
1	A	512	HIS
1	A	533	ASN
1	A	536	ASN

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Mol	Chain	Res	Type
1	A	548	GLN
1	A	561	ASN
1	A	562	ASN
1	A	577	GLN
1	A	617	GLN
1	A	620	ASN
1	A	661	ASN
1	A	668	ASN
1	A	696	GLN
1	A	698	ASN
1	A	703	GLN
1	A	709	GLN
1	A	732	ASN
1	A	742	GLN
1	A	748	ASN
1	A	788	ASN
1	A	812	ASN
1	A	820	ASN
1	A	821	ASN
1	A	854	ASN
1	A	871	ASN
1	A	886	ASN
1	A	903	ASN
1	A	914	ASN
1	A	925	ASN
1	A	932	ASN
1	A	941	ASN
1	A	957	ASN
1	A	964	GLN
1	A	997	ASN
1	A	1019	ASN
1	A	1035	ASN
1	A	1048	ASN
1	A	1065	ASN
1	A	1068	ASN
1	A	1109	ASN
1	A	1138	ASN
1	A	1147	GLN
1	A	1185	ASN
1	A	1196	ASN
1	A	1241	ASN
1	B	5	ASN

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	95	ASN
1	B	111	ASN
1	B	116	ASN
1	B	125	HIS
1	B	175	ASN
1	B	197	ASN
1	B	200	ASN
1	B	290	GLN
1	B	349	GLN
1	B	370	ASN
1	B	378	ASN
1	B	383	ASN
1	B	444	ASN
1	B	470	GLN
1	B	474	ASN
1	B	512	HIS
1	B	561	ASN
1	B	562	ASN
1	B	568	GLN
1	B	589	GLN
1	B	617	GLN
1	B	620	ASN
1	B	661	ASN
1	B	668	ASN
1	B	696	GLN
1	B	698	ASN
1	B	703	GLN
1	B	706	GLN
1	B	709	GLN
1	B	788	ASN
1	B	799	GLN
1	B	812	ASN
1	B	821	ASN
1	B	854	ASN
1	B	884	ASN
1	B	886	ASN
1	B	903	ASN
1	B	925	ASN
1	B	941	ASN
1	B	957	ASN
1	B	964	GLN

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Mol	Chain	Res	Type
1	B	966	ASN
1	B	981	ASN
1	B	997	ASN
1	B	1014	GLN
1	B	1048	ASN
1	B	1065	ASN
1	B	1070	ASN
1	B	1096	ASN
1	B	1130	GLN
1	B	1133	ASN
1	B	1170	ASN
1	B	1185	ASN
1	B	1196	ASN
1	B	1204	ASN
1	B	1241	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	A	1303	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-
4	ACT	B	1303	-	1,3,3	3.07	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACT	A	1303	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1303	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1303	ACT	CH3-C	2.26	1.51	1.48
4	B	1303	ACT	CH3-C	3.07	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1246/1252 (99%)	-0.07	50 (4%)	38	34	12, 45, 86, 109	0
1	B	1238/1252 (98%)	0.24	81 (6%)	19	16	24, 62, 96, 109	0
All	All	2484/2504 (99%)	0.09	131 (5%)	26	23	12, 53, 93, 109	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	655	GLY	8.7
1	A	477	SER	8.6
1	B	477	SER	7.9
1	A	655	GLY	7.6
1	A	657	SER	6.6
1	A	656	SER	6.3
1	B	654	LEU	6.0
1	B	656	SER	6.0
1	B	479	SER	5.7
1	B	570	ALA	5.5
1	B	291	VAL	5.3
1	B	831	THR	5.2
1	A	476	ASN	5.1
1	A	740	ILE	4.9
1	B	735	THR	4.9
1	B	569	ALA	4.8
1	B	657	SER	4.7
1	B	740	ILE	4.6
1	A	498	ILE	4.6
1	A	658	ASP	4.5
1	B	833	ASP	4.5
1	B	847	ILE	4.5
1	A	1232	HIS	4.4
1	A	567	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	654	LEU	4.3
1	B	929	LYS	4.3
1	B	969	ILE	4.2
1	B	658	ASP	4.2
1	B	1138	ASN	4.1
1	B	478	GLU	4.1
1	B	912	TYR	3.9
1	B	834	LYS	3.8
1	B	290	GLN	3.8
1	A	833	ASP	3.8
1	B	498	ILE	3.8
1	A	479	SER	3.8
1	B	738	TYR	3.7
1	B	492	ILE	3.7
1	A	482	GLY	3.6
1	B	729	GLU	3.6
1	B	459	THR	3.5
1	B	380	LEU	3.5
1	B	1230	ARG	3.5
1	B	726	TYR	3.5
1	B	147	ASN	3.4
1	B	182	ALA	3.4
1	A	328	PHE	3.3
1	B	475	PHE	3.2
1	B	835	ILE	3.2
1	B	802	SER	3.2
1	B	148	VAL	3.2
1	B	1232	HIS	3.2
1	A	453	GLU	3.2
1	A	929	LYS	3.2
1	A	836	LEU	3.2
1	B	719	ILE	3.1
1	A	198	CYS	3.1
1	A	834	LYS	3.1
1	B	480	ALA	3.1
1	A	419	LYS	3.1
1	A	735	THR	3.1
1	A	831	THR	3.0
1	A	1233	THR	3.0
1	B	448	ILE	3.0
1	B	946	ASN	2.9
1	A	1169	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	728	LEU	2.9
1	A	1231	ASP	2.9
1	A	308	GLY	2.9
1	B	832	ASP	2.8
1	B	146	PRO	2.8
1	B	10	ASN	2.8
1	B	734	LEU	2.8
1	A	418	VAL	2.8
1	A	478	GLU	2.7
1	B	149	ILE	2.7
1	A	119	THR	2.7
1	A	459	THR	2.7
1	A	475	PHE	2.7
1	B	328	PHE	2.7
1	B	572	PHE	2.6
1	B	1137	THR	2.6
1	A	728	LEU	2.6
1	A	457	THR	2.5
1	A	832	ASP	2.5
1	B	744	GLU	2.5
1	A	483	LEU	2.5
1	A	492	ILE	2.5
1	A	199	MET	2.5
1	B	836	LEU	2.5
1	B	491	THR	2.4
1	B	731	LYS	2.4
1	A	835	ILE	2.4
1	A	310	ASP	2.4
1	B	300	LYS	2.4
1	B	806	GLU	2.4
1	B	110	ALA	2.4
1	B	1076	TRP	2.4
1	A	912	TYR	2.3
1	B	910	ASN	2.3
1	B	1049	ILE	2.3
1	B	1231	ASP	2.3
1	A	1230	ARG	2.3
1	A	196	ASP	2.3
1	B	741	LYS	2.3
1	B	145	LEU	2.3
1	A	1250	GLN	2.3
1	B	653	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	455	ASP	2.2
1	B	567	VAL	2.2
1	A	1136	SER	2.2
1	B	162	SER	2.2
1	B	830	TYR	2.2
1	B	181	ILE	2.2
1	A	290	GLN	2.2
1	B	1133	ASN	2.2
1	B	565	LYS	2.2
1	A	448	ILE	2.1
1	B	130	SER	2.1
1	B	837	ILE	2.1
1	B	120	PRO	2.1
1	A	493	GLN	2.1
1	A	847	ILE	2.1
1	B	39	ILE	2.1
1	B	289	VAL	2.1
1	B	828	SER	2.1
1	A	729	GLU	2.1
1	B	112	PRO	2.0
1	B	111	ASN	2.0
1	B	663	VAL	2.0
1	B	490	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	A	1303	4/4	0.75	0.29	70,70,71,71	0
4	ACT	B	1303	4/4	0.81	0.20	65,65,66,66	0
3	NA	A	1301	1/1	0.96	0.08	62,62,62,62	0
3	NA	B	1302	1/1	0.96	0.08	55,55,55,55	0
3	NA	A	1302	1/1	0.98	0.07	38,38,38,38	0
2	ZN	B	1300	1/1	0.99	0.04	47,47,47,47	0
2	ZN	A	1300	1/1	0.99	0.10	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.