



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:24 am BST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

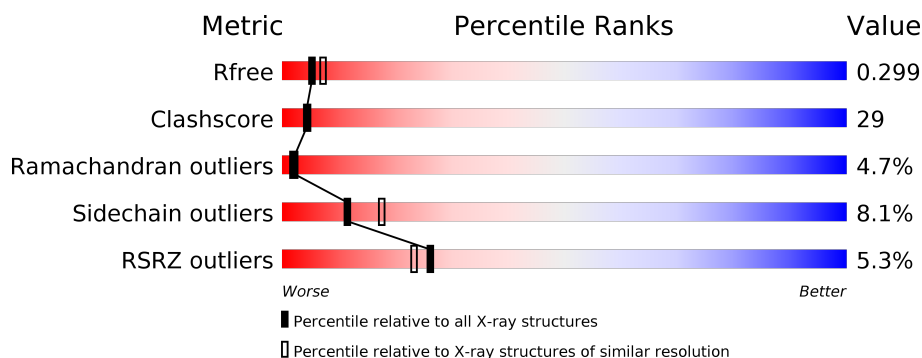
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1252	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>39%</div> <div>7%</div> </div> <div>•</div> </div>
1	B	1252	<div> <div>6%</div> <div> <div></div> <div>47%</div> <div>45%</div> <div>6%</div> </div> <div>••</div> </div>

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

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

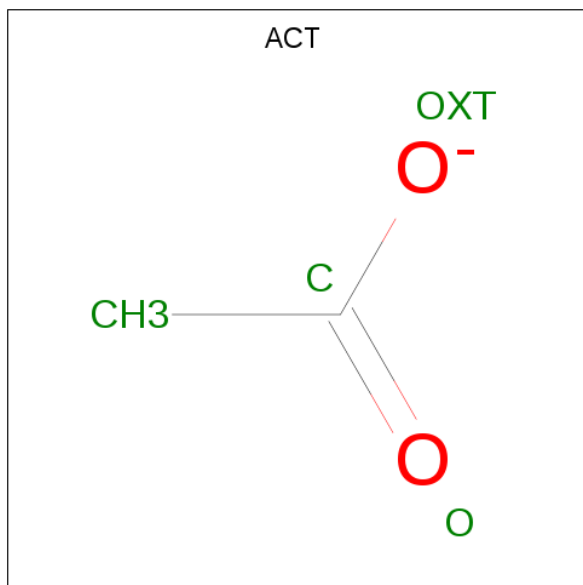
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

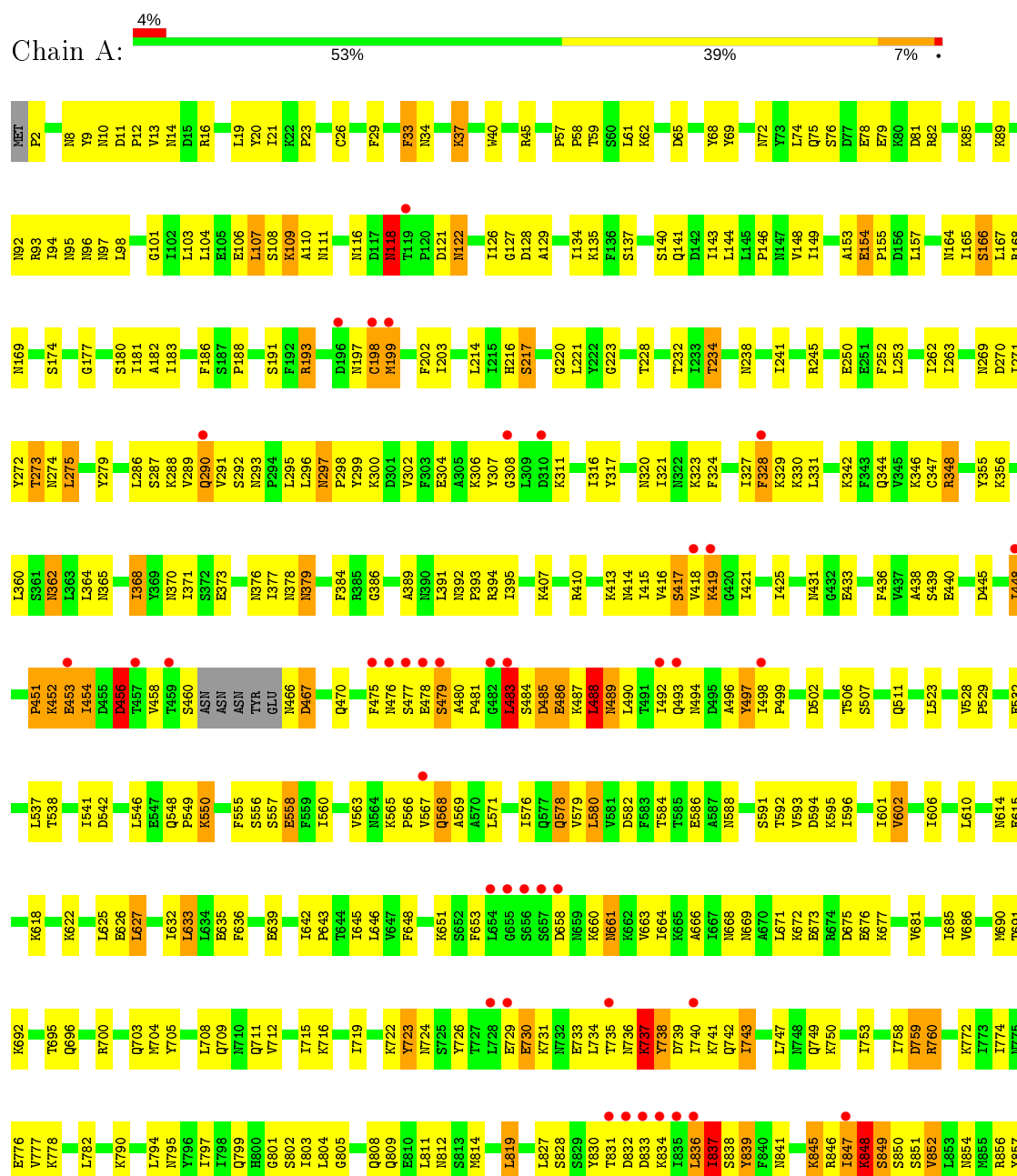
- Molecule 5 is water.

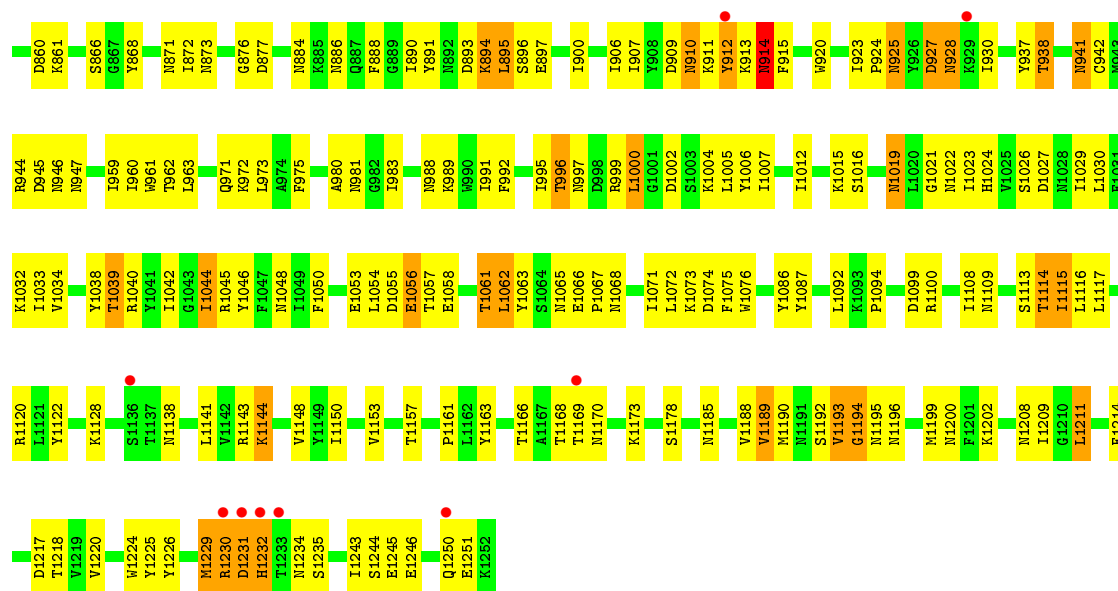
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	62	Total O 62 62	0	0
5	B	32	Total O 32 32	0	0

### 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 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: Botulinum neurotoxin type E





Q1250	T1169	P1094	K1015	D860	Y785	N713	F636
E1251	N1170	N1095	S1016	D864	N788	A714	E639
K1252	K1171	N1096	L1020	Y868	Y789	I715	L640
	S1178	F1097	G1021	Y872	L793	I717	L641
	R1183	I1098	N1022	I873	L794	I718	L642
	F1184	D1099	I1023	I874	N795	I719	L646
	N1185	R1100	D1027	I875	Y796	E720	
	Q1186	K1102	N1028	N876	I797	Y723	T649
	V1187	D1103	I1029	G876	I798	N724	I650
	V1188	S1104	L1030	D877	Q799	S725	
	V1189	F1031	F1030	V878	B800	Y726	F653
	M1190	K1032	K1032	Y879	G801	T727	L694
	N1191	I1108	I1033	N884	S802	L728	G654
	S1192	F1034	V1034	K885	L804	E729	S656
	V1193	N1035	N1035	N886	G805	E730	S657
	G1194	Y1038	Y1038	Q887	E806	K731	D658
	N1195	T1039	T1039	F888	Q809	N732	N659
	M1199	R1040	R1040	G889	L734	E733	K660
	N1200	Y1041	Y1041	I890	N812	T735	N661
	F1201	L1116	Q964	Y891	N813	N736	K662
	K1202	L1117	D965	N892	S813	K737	V663
	N1203	L1121	I966	D893	N814	Y738	
	N1204	L1126	A967	K894	T819	D739	A666
	N1205	K1126	G968	L895	F825	I740	I667
	G1206	Q1130	N969	S896	K741	K741	N668
	N1207	N1049	I970	E897	Q742	N669	N669
	N1208	R1131	Q971	V898	I743	A670	L671
	I1209	V1132	K972	N899	E744	K672	
	G1210	N1133	L973	I900	S828	N745	
	L1211	N1134	N979	N903	S829	I746	D675
	K1215	S1135	A980	D904	Y830	E747	E676
	A1216	T1137	N981	Y905	D832	N748	K677
		N1138	G982	I906	D833	Q749	W678
		D1139	N983	I907	K834	K750	
	W1224	N1140	Y886	N910	L835	V751	V681
	Y1225	L1141	Y912	K911	L836	S752	
	Y1226	V1142	Y912	Y912	I837	I753	T685
	T1227	R1143	Y912	Y912	S838	A754	T691
	H1228	K1144	T994	K913	F840	I758	K692
	M1229		I995	N914	N841	D759	I693
	R1230	V1148	T996	F915	K842	F761	K694
	D1231	I1149		S916	F843	Q696	
	H1232	N1151	R999	F919		L762	
	T1233	F1152	L1000	W920	R846	R700	R700
	N1234	V1153	G1001	V921	K848	K701	K701
	S1235	T1157	D1002	R922	S849	E702	E702
	F1239	H1158	S1003	I923	S850	Q703	Q703
	W1240		K1004	P924	S851	M704	M704
	N1241	P1161	L1005	N925	V852	Y705	Y705
	F1242	L1162	Y1006	Y926	L853	Q706	Q706
	I1243	T1166	I1007	D827	N854	A707	A707
	S1244	A1167	I1012	N928	K855		
	E1245	T1168	D1013	R929	R856	N710	N710
	E1246		Q1014	I930	Y857	Q711	Q711
	W1249					L782	V712



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.253 , 0.309 0.244 , 0.299	Depositor DCC
$R_{free}$ test set	4751 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality [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(°)	Ideal(°)
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(°)	Ideal(°)
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 ⓘ

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 ⓘ

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%)	11	16
1	B	1139/1153 (99%)	1051 (92%)	88 (8%)	13	20
All	All	2285/2306 (99%)	2101 (92%)	184 (8%)	11	17

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 ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	B	1303	-	1,3,3	3.07	1 (100%)	0,3,3	0.00	-
4	ACT	A	1303	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1303	ACT	CH3-C	3.07	1.52	1.48
4	A	1303	ACT	CH3-C	2.26	1.51	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1246/1252 (99%)	-0.07	50 (4%)	38	34	12, 45, 86, 109	0
1	B	1238/1252 (98%)	0.24	81 (6%)	18	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	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.