



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:06 am GMT

PDB ID : 2Q5D  
Title : Crystal Structure of Human Importin Beta bound to the Snurportin1 IBB-domain second crystal form  
Authors : Mitrousis, G.; Cingolani, G.  
Deposited on : 2007-05-31  
Resolution : 3.20 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

<http://wwpdb.org/validation/2016/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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

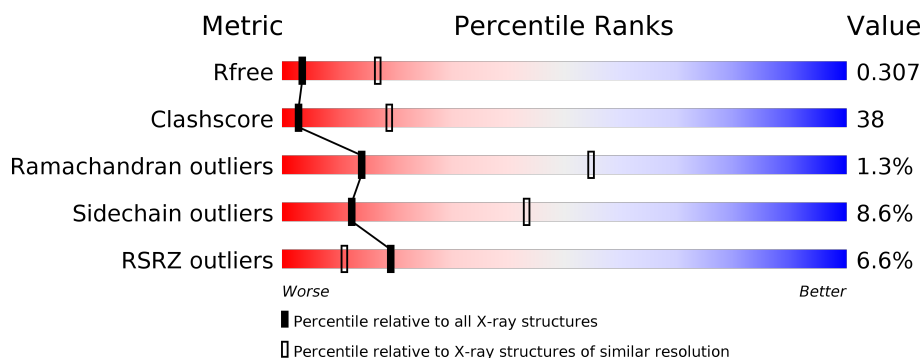
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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. 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	876	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>33%</div> <div>5% ..</div> </div> </div>
1	B	876	<div> <div>10%</div> <div> <div></div> <div>51%</div> <div>33%</div> <div>11% . .</div> </div> </div>
2	C	40	<div> <div></div> <div> <div></div> <div>50%</div> <div>30%</div> <div>10%</div> <div>10%</div> </div> </div>
2	D	40	<div> <div>10%</div> <div> <div></div> <div>48%</div> <div>10%</div> <div>43%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13750 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 Importin beta-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	871	Total	C	N	O	S	1	0	0
			6762	4259	1135	1321	47			
1	B	845	Total	C	N	O	S	0	0	0
			6550	4129	1100	1275	46			

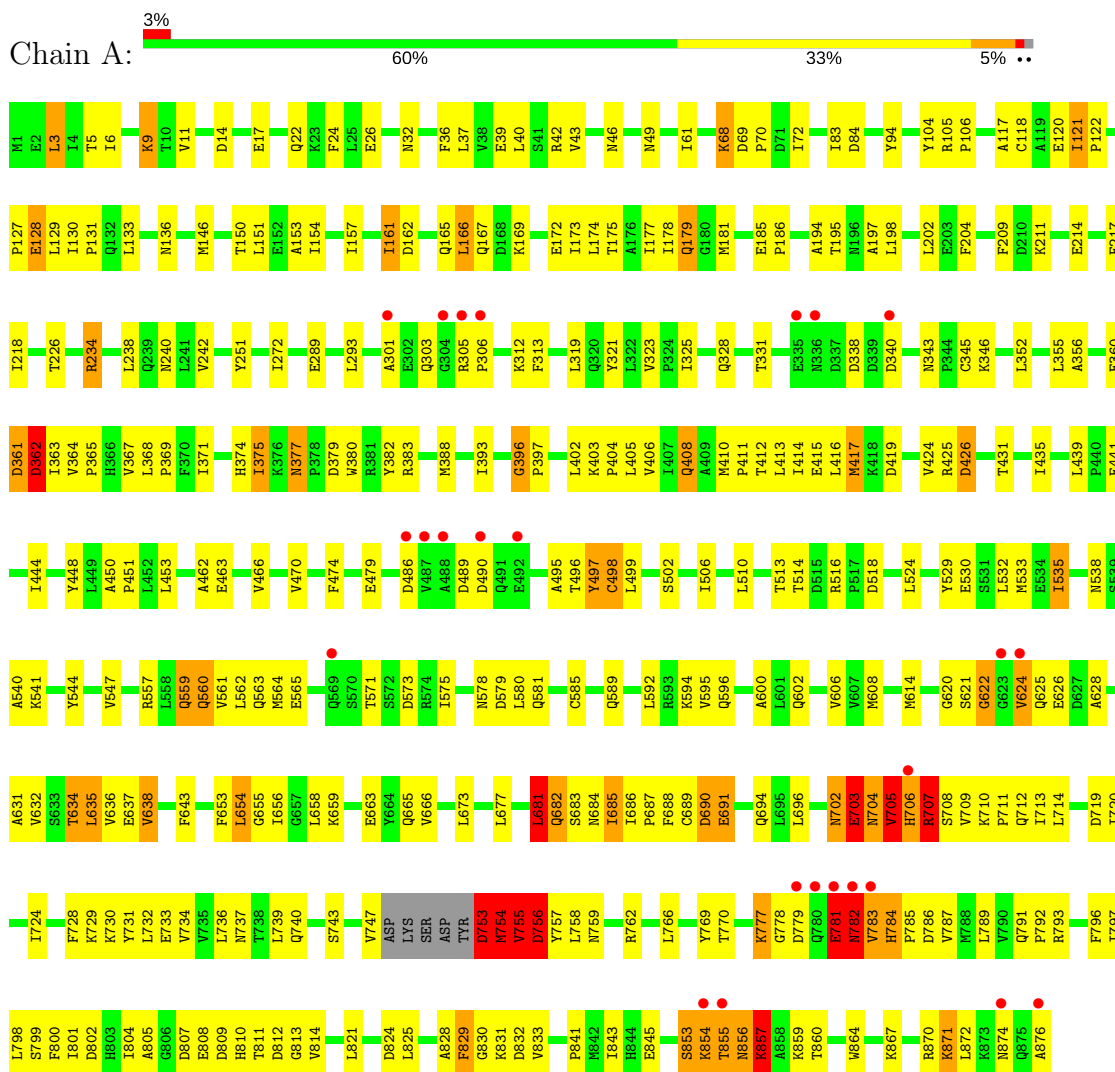
- Molecule 2 is a protein called Snurportin-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	36	Total	C	N	O	0	0	0
			323	198	70	55			
2	D	23	Total	C	N	O	0	0	0
			115	69	23	23			

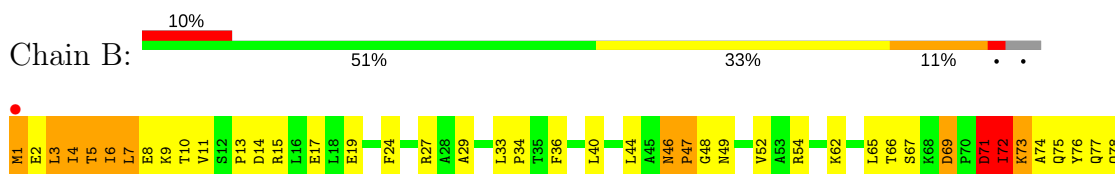
### 3 Residue-property plots

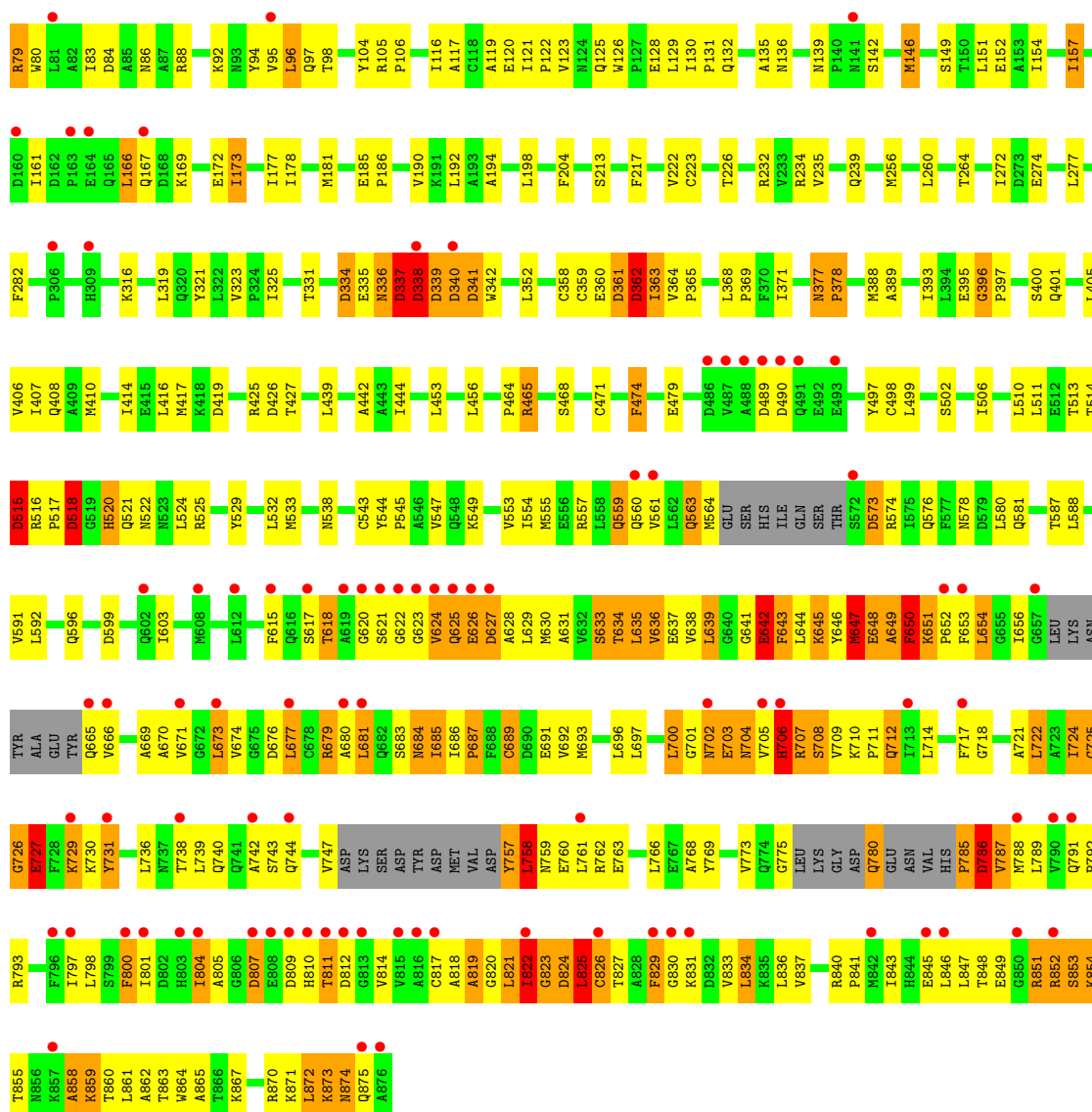
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Importin beta-1 subunit

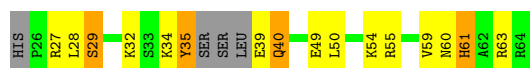


#### • Molecule 1: Importin beta-1 subunit

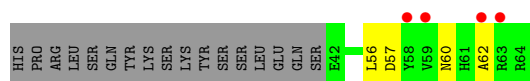




• Molecule 2: Snurportin-1



• Molecule 2: Snurportin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.98Å 100.70Å 108.68Å 90.00° 109.23° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 39.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 91.3 (39.61-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.303 , 0.328 0.296 , 0.307	Depositor DCC
$R_{free}$ test set	1598 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.4	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 73.8	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	0.87	EDS
Total number of atoms	13750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.47	0/6871	0.68	11/9328 (0.1%)
1	B	0.42	0/6651	0.67	19/9023 (0.2%)
2	C	0.50	0/326	0.67	0/428
2	D	0.47	0/114	0.37	0/158
All	All	0.44	0/13962	0.67	30/18937 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	25
1	B	0	48
All	All	0	73

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	396	GLY	C-N-CD	-5.68	108.11	120.60
1	A	779	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	690	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	832	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	337	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	362	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	824	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	786	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	339	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	426	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	812	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	361	ASP	CB-CG-OD2	5.25	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	518	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	341	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	573	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	579	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	753	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	786	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	334	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	69	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	756	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	362	ASP	CB-CG-OD2	5.21	122.98	118.30
1	B	809	ASP	CB-CG-OD2	5.21	122.98	118.30
1	B	812	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	361	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	71	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	573	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	338	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	515	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

All (73) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	TYR	Peptide
1	A	396	GLY	Peptide
1	A	498	CYS	Peptide
1	A	622	GLY	Peptide
1	A	681	LEU	Peptide
1	A	702	ASN	Peptide
1	A	703	GLU	Peptide
1	A	704	ASN	Peptide
1	A	705	VAL	Peptide
1	A	706	HIS	Peptide
1	A	707	ARG	Peptide
1	A	753	ASP	Peptide
1	A	754	MET	Peptide
1	A	777	LYS	Peptide
1	A	781	GLU	Peptide
1	A	782	ASN	Peptide
1	A	783	VAL	Peptide
1	A	784	HIS	Peptide
1	A	828	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	829	PHE	Peptide
1	A	830	GLY	Peptide
1	A	853	SER	Peptide
1	A	854	LYS	Peptide
1	A	857	LYS	Peptide
1	A	871	LYS	Peptide
1	B	1	MET	Peptide
1	B	3	LEU	Peptide
1	B	335	GLU	Peptide
1	B	336	ASN	Peptide
1	B	337	ASP	Peptide
1	B	338	ASP	Peptide
1	B	363	ILE	Peptide
1	B	46	ASN	Peptide
1	B	48	GLY	Peptide
1	B	517	PRO	Peptide
1	B	518	ASP	Peptide
1	B	520	HIS	Peptide
1	B	521	GLN	Peptide
1	B	596	GLN	Peptide
1	B	6	ILE	Peptide
1	B	623	GLY	Peptide
1	B	639	LEU	Peptide
1	B	642	GLU	Peptide
1	B	643	PHE	Peptide
1	B	647	MET	Peptide
1	B	648	GLU	Peptide
1	B	649	ALA	Peptide
1	B	650	PHE	Peptide
1	B	654	LEU	Peptide
1	B	656	ILE	Peptide
1	B	679	ARG	Peptide
1	B	684	ASN	Peptide
1	B	701	GLY	Peptide
1	B	702	ASN	Peptide
1	B	703	GLU	Peptide
1	B	706	HIS	Peptide
1	B	72	ILE	Peptide
1	B	724	ILE	Peptide
1	B	725	GLY	Peptide
1	B	726	GLY	Peptide
1	B	727	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	729	LYS	Peptide
1	B	758	LEU	Peptide
1	B	785	PRO	Peptide
1	B	786	ASP	Peptide
1	B	821	LEU	Peptide
1	B	822	ILE	Peptide
1	B	823	GLY	Peptide
1	B	825	LEU	Peptide
1	B	826	CYS	Peptide
1	B	858	ALA	Peptide
1	B	874	ASN	Peptide
1	B	875	GLN	Peptide

## 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	6762	0	6764	426	0
1	B	6550	0	6568	655	0
2	C	323	0	337	15	0
2	D	115	0	48	6	0
All	All	13750	0	13717	1047	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 38.

All (1047) 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:686:ILE:CG1	1:B:687:PRO:HD3	1.08	1.56
1:B:686:ILE:CG1	1:B:687:PRO:CD	2.02	1.37
1:B:647:MET:CA	1:B:649:ALA:HB2	1.52	1.35
1:B:647:MET:SD	1:B:649:ALA:HB3	1.65	1.35
1:A:130:ILE:CG2	1:A:131:PRO:HD3	1.61	1.30
1:A:778:GLY:HA3	1:A:781:GLU:OE2	1.24	1.30
1:B:686:ILE:HG13	1:B:687:PRO:CD	1.58	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:MET:SD	1:B:649:ALA:CB	2.21	1.28
1:A:782:ASN:HB3	1:B:574:ARG:CB	1.65	1.25
1:B:3:LEU:HD13	1:B:24:PHE:CE1	1.72	1.23
1:B:705:VAL:O	1:B:707:ARG:HB3	1.39	1.21
1:B:647:MET:HA	1:B:649:ALA:CB	1.70	1.21
1:B:3:LEU:O	1:B:6:ILE:HG22	1.45	1.16
1:A:781:GLU:O	1:B:573:ASP:HB2	1.41	1.15
1:A:562:LEU:HD23	1:A:562:LEU:O	1.46	1.15
1:A:782:ASN:CB	1:B:574:ARG:HB2	1.78	1.14
1:B:3:LEU:CD1	1:B:24:PHE:CE1	2.30	1.14
1:B:130:ILE:CG1	1:B:131:PRO:HD3	1.78	1.14
1:B:130:ILE:CG1	1:B:131:PRO:CD	2.25	1.14
1:A:130:ILE:HG23	1:A:131:PRO:CD	1.76	1.13
1:A:561:VAL:HA	1:A:564:MET:HG3	1.25	1.12
1:A:130:ILE:CG2	1:A:131:PRO:CD	2.27	1.12
1:A:704:ASN:HB2	1:A:705:VAL:HG22	1.23	1.12
1:B:3:LEU:HB3	1:B:6:ILE:HG21	1.23	1.11
1:B:130:ILE:HG13	1:B:131:PRO:HD3	1.13	1.10
1:B:819:ALA:HA	1:B:822:ILE:CG2	1.80	1.10
1:B:821:LEU:HD13	1:B:821:LEU:O	1.50	1.10
1:B:848:THR:HA	1:B:851:ARG:HE	1.14	1.09
1:B:130:ILE:HG13	1:B:131:PRO:CD	1.81	1.09
1:B:69:ASP:HB2	1:B:72:ILE:CG2	1.82	1.09
1:B:96:LEU:HD21	1:B:132:GLN:HG2	1.23	1.08
1:A:737:ASN:HD22	1:B:13:PRO:HA	0.92	1.08
1:A:777:LYS:HG2	1:A:778:GLY:H	1.12	1.08
1:B:721:ALA:HA	1:B:724:ILE:HG22	1.36	1.08
1:B:681:LEU:HD13	1:B:685:ILE:CG2	1.83	1.07
1:B:647:MET:C	1:B:649:ALA:HB2	1.73	1.07
1:B:634:THR:O	1:B:638:VAL:HG23	1.51	1.07
1:B:686:ILE:HG12	1:B:687:PRO:HD3	1.13	1.05
1:A:782:ASN:HB3	1:B:574:ARG:HB2	1.05	1.04
1:B:1:MET:HB2	1:B:3:LEU:HG	1.36	1.04
1:B:681:LEU:HD13	1:B:685:ILE:HG22	1.04	1.03
1:A:783:VAL:O	1:A:785:PRO:HD3	1.58	1.03
1:B:819:ALA:C	1:B:822:ILE:HG23	1.78	1.03
1:B:69:ASP:HB2	1:B:72:ILE:HG23	1.38	1.03
1:A:783:VAL:C	1:A:785:PRO:HD3	1.78	1.02
1:A:870:ARG:CZ	1:B:342:TRP:HD1	1.73	1.02
1:A:704:ASN:CB	1:A:705:VAL:HG22	1.89	1.01
1:B:592:LEU:CD1	1:B:638:VAL:HG11	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:819:ALA:CA	1:B:822:ILE:CG2	2.37	1.01
1:A:118:CYS:HA	1:A:161:ILE:HD12	1.41	1.01
1:A:130:ILE:HG23	1:A:131:PRO:HD3	1.03	1.00
1:B:1:MET:HB3	1:B:2:GLU:O	1.61	1.00
1:B:811:THR:HG23	1:B:814:VAL:HG23	1.38	1.00
1:A:737:ASN:ND2	1:B:13:PRO:HA	1.76	1.00
1:B:651:LYS:HD3	1:B:691:GLU:HB3	1.43	1.00
1:A:867:LYS:HG3	1:B:341:ASP:OD1	1.61	0.99
1:B:105:ARG:HB2	1:B:106:PRO:HD3	1.45	0.99
1:B:686:ILE:HG12	1:B:687:PRO:CD	1.75	0.99
1:B:826:CYS:SG	1:B:865:ALA:HA	2.02	0.99
1:B:707:ARG:HG2	1:B:757:TYR:CE1	1.97	0.99
1:A:870:ARG:HH21	1:B:277:LEU:HD22	1.27	0.99
1:B:762:ARG:HH11	1:B:800:PHE:HD1	1.00	0.99
1:B:130:ILE:HG12	1:B:131:PRO:HD2	1.41	0.99
1:B:3:LEU:HD11	1:B:24:PHE:CZ	1.96	0.98
1:A:686:ILE:HA	1:A:689:CYS:SG	2.03	0.98
1:A:755:VAL:CG2	1:A:756:ASP:H	1.76	0.98
1:B:822:ILE:HD11	1:B:861:LEU:HB2	1.43	0.98
1:A:755:VAL:HG23	1:A:756:ASP:H	1.25	0.98
1:B:685:ILE:H	1:B:685:ILE:HD13	1.28	0.98
1:B:819:ALA:C	1:B:822:ILE:CG2	2.31	0.98
1:B:647:MET:HA	1:B:649:ALA:HB2	0.99	0.98
1:A:784:HIS:N	1:A:785:PRO:HD3	1.79	0.97
1:B:848:THR:HA	1:B:851:ARG:NE	1.78	0.97
1:A:737:ASN:HD22	1:B:13:PRO:CA	1.75	0.97
1:B:641:GLY:O	1:B:642:GLU:HG3	1.65	0.97
1:B:3:LEU:HB3	1:B:6:ILE:CG2	1.93	0.96
1:B:3:LEU:HD13	1:B:24:PHE:HE1	1.28	0.96
1:B:169:LYS:O	1:B:173:ILE:HD13	1.66	0.95
1:B:592:LEU:HD13	1:B:638:VAL:HG11	1.44	0.95
1:B:1:MET:HB2	1:B:3:LEU:CG	1.96	0.95
1:A:777:LYS:HG2	1:A:778:GLY:N	1.79	0.95
1:B:679:ARG:HH11	1:B:679:ARG:HG3	1.30	0.95
1:A:755:VAL:CG2	1:A:756:ASP:N	2.30	0.95
1:B:130:ILE:HG12	1:B:131:PRO:CD	1.94	0.95
1:A:356:ALA:HA	1:A:363:ILE:HD13	1.49	0.94
1:B:852:ARG:HG3	1:B:852:ARG:HH11	1.31	0.94
2:C:34:LYS:O	2:C:35:TYR:HB2	1.62	0.94
1:B:819:ALA:HA	1:B:822:ILE:HG22	1.47	0.94
1:B:766:LEU:HB3	1:B:821:LEU:HD23	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ILE:HD13	1:A:375:ILE:O	1.67	0.93
1:B:644:LEU:O	1:B:644:LEU:HD12	1.68	0.93
1:B:649:ALA:HA	1:B:650:PHE:CD2	2.03	0.93
1:B:848:THR:HG23	1:B:851:ARG:HH21	1.31	0.92
1:B:801:ILE:HG21	1:B:846:LEU:HD22	1.50	0.92
1:B:644:LEU:HB2	1:B:684:ASN:OD1	1.70	0.92
1:B:759:ASN:HD22	1:B:814:VAL:CA	1.84	0.91
1:B:827:THR:OG1	1:B:864:TRP:CH2	2.23	0.91
1:B:647:MET:CA	1:B:649:ALA:CB	2.39	0.91
1:B:712:GLN:HA	1:B:712:GLN:HE21	1.34	0.91
1:B:811:THR:HG23	1:B:814:VAL:CG2	1.99	0.91
1:B:787:VAL:HB	1:B:789:LEU:CG	2.01	0.91
1:B:693:MET:HG2	1:B:731:TYR:OH	1.70	0.91
1:B:762:ARG:HD2	1:B:800:PHE:CD1	2.05	0.91
1:A:870:ARG:NH2	1:B:342:TRP:HD1	1.69	0.90
1:B:762:ARG:NH1	1:B:800:PHE:HD1	1.68	0.90
1:A:782:ASN:HB3	1:B:574:ARG:CA	2.02	0.89
1:B:1:MET:HG3	1:B:3:LEU:HD21	1.53	0.89
1:B:105:ARG:CB	1:B:106:PRO:HD3	2.02	0.89
1:B:647:MET:SD	1:B:649:ALA:HB1	2.09	0.89
1:B:3:LEU:CD1	1:B:24:PHE:HE1	1.82	0.89
1:B:339:ASP:O	1:B:340:ASP:HB2	1.73	0.89
1:B:787:VAL:HB	1:B:789:LEU:CD1	2.03	0.89
1:A:720:ILE:HG23	1:A:724:ILE:HD13	1.55	0.88
1:A:3:LEU:HA	1:A:6:ILE:CD1	2.04	0.88
1:B:727:GLU:H	1:B:727:GLU:CD	1.75	0.88
1:B:11:VAL:HG21	1:B:52:VAL:HG11	1.54	0.88
1:B:825:LEU:HD23	1:B:825:LEU:N	1.89	0.88
1:B:833:VAL:HG12	1:B:837:VAL:HG23	1.56	0.88
1:A:704:ASN:HB2	1:A:705:VAL:CG2	2.04	0.88
1:B:721:ALA:HA	1:B:724:ILE:CG2	2.02	0.87
1:B:759:ASN:ND2	1:B:814:VAL:HA	1.87	0.87
1:B:759:ASN:HD22	1:B:814:VAL:HA	1.38	0.87
1:B:743:SER:HA	1:B:762:ARG:NH2	1.89	0.87
1:A:589:GLN:HG2	1:A:634:THR:HG21	1.54	0.87
1:B:693:MET:CG	1:B:731:TYR:OH	2.23	0.87
1:A:831:LYS:HB2	1:A:872:LEU:HD22	1.57	0.87
1:A:871:LYS:HG2	1:B:340:ASP:HA	1.56	0.87
1:B:516:ARG:NH2	1:B:524:LEU:HD13	1.89	0.86
1:B:5:THR:O	1:B:5:THR:HG22	1.72	0.86
1:B:671:VAL:HG11	1:B:709:VAL:HG13	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ALA:HA	1:A:363:ILE:CD1	2.05	0.86
1:B:651:LYS:HD3	1:B:691:GLU:CB	2.06	0.86
1:A:343:ASN:HD21	1:A:345:CYS:HB3	1.37	0.86
1:A:781:GLU:O	1:B:573:ASP:CB	2.24	0.86
1:B:722:LEU:CD1	2:D:62:ALA:HB1	2.05	0.86
1:A:360:GLU:HG2	1:A:396:GLY:O	1.76	0.85
1:B:377:ASN:HD22	1:B:378:PRO:CD	1.89	0.85
1:A:705:VAL:HG12	1:A:706:HIS:HB2	1.57	0.85
1:A:3:LEU:HA	1:A:6:ILE:HD11	1.57	0.85
1:B:1:MET:CB	1:B:3:LEU:HG	2.06	0.85
1:B:787:VAL:HB	1:B:789:LEU:HG	1.58	0.85
1:B:27:ARG:HG3	1:B:27:ARG:HH11	1.42	0.85
1:B:830:GLY:HA3	1:B:872:LEU:HG	1.56	0.85
1:A:130:ILE:HG22	1:A:131:PRO:HD3	1.59	0.84
1:B:555:MET:SD	1:B:603:ILE:HG12	2.18	0.84
1:B:516:ARG:HH22	1:B:524:LEU:HD13	1.40	0.84
1:B:759:ASN:HD22	1:B:814:VAL:HG13	1.41	0.84
1:B:3:LEU:HD11	1:B:24:PHE:CE1	2.10	0.84
1:A:561:VAL:HA	1:A:564:MET:CG	2.06	0.84
1:B:766:LEU:HD13	1:B:821:LEU:HB2	1.59	0.83
1:B:759:ASN:ND2	1:B:814:VAL:HG13	1.93	0.83
1:A:831:LYS:HE2	1:A:876:ALA:HB3	1.59	0.83
1:B:573:ASP:HA	1:B:576:GLN:HB2	1.58	0.83
1:B:762:ARG:NH1	1:B:800:PHE:CD1	2.45	0.83
1:A:870:ARG:NH2	1:B:342:TRP:CD1	2.46	0.83
1:A:130:ILE:HG22	1:A:131:PRO:CD	2.07	0.82
1:A:685:ILE:HD13	1:A:688:PHE:HB2	1.61	0.82
1:B:1:MET:HE2	1:B:3:LEU:HD23	1.60	0.82
1:B:840:ARG:HB3	1:B:843:ILE:HD13	1.59	0.82
1:B:154:ILE:HA	1:B:157:ILE:HD12	1.62	0.82
1:A:343:ASN:ND2	1:A:345:CYS:HB3	1.94	0.82
1:A:498:CYS:O	1:A:499:LEU:HD23	1.79	0.82
1:B:644:LEU:HD13	1:B:684:ASN:HD21	1.45	0.82
1:B:759:ASN:HD22	1:B:814:VAL:CG1	1.91	0.81
1:A:178:ILE:HD12	1:A:217:PHE:CE2	2.14	0.81
1:B:395:GLU:O	1:B:397:PRO:HD3	1.79	0.81
1:B:3:LEU:CD1	1:B:24:PHE:CZ	2.60	0.81
1:A:856:ASN:C	1:A:857:LYS:HG2	2.00	0.81
1:B:515:ASP:HB2	1:B:557:ARG:NH2	1.96	0.81
1:B:377:ASN:HD22	1:B:378:PRO:N	1.78	0.81
1:B:818:ALA:O	1:B:846:LEU:HD21	1.82	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:826:CYS:SG	1:B:865:ALA:CA	2.68	0.81
1:A:706:HIS:CD2	1:A:706:HIS:O	2.34	0.80
1:B:644:LEU:CD1	1:B:684:ASN:HD21	1.94	0.80
1:B:787:VAL:HB	1:B:789:LEU:HD11	1.62	0.80
1:B:852:ARG:HG3	1:B:852:ARG:NH1	1.96	0.80
1:A:561:VAL:HG22	1:A:564:MET:CE	2.12	0.80
1:B:5:THR:CG2	1:B:5:THR:O	2.30	0.80
1:B:693:MET:SD	1:B:731:TYR:OH	2.40	0.80
1:B:377:ASN:HD22	1:B:378:PRO:HD2	1.47	0.80
1:A:377:ASN:HD22	1:A:379:ASP:H	1.29	0.79
1:A:665:GLN:OE1	1:A:665:GLN:HA	1.81	0.79
1:B:65:LEU:HD21	1:B:80:TRP:CD2	2.19	0.78
1:A:783:VAL:O	1:A:785:PRO:CD	2.31	0.78
1:A:778:GLY:HA3	1:A:781:GLU:CD	2.04	0.78
1:A:755:VAL:HG22	1:A:756:ASP:N	1.97	0.78
1:B:804:ILE:HD12	1:B:814:VAL:HG11	1.65	0.78
1:A:829:PHE:O	1:A:833:VAL:HG23	1.84	0.78
1:A:37:LEU:HD23	1:A:61:ILE:HD13	1.63	0.78
1:B:647:MET:C	1:B:649:ALA:CB	2.53	0.78
1:A:870:ARG:NH2	1:B:277:LEU:HD22	1.98	0.77
1:A:560:GLN:O	1:A:564:MET:HG3	1.84	0.77
1:A:154:ILE:HA	1:A:157:ILE:HD12	1.66	0.77
1:B:711:PRO:HD3	1:B:757:TYR:OH	1.84	0.77
1:B:819:ALA:HA	1:B:822:ILE:HG21	1.67	0.77
1:A:782:ASN:HA	1:B:574:ARG:H	1.50	0.77
1:B:722:LEU:HD13	2:D:62:ALA:HB1	1.66	0.76
1:B:822:ILE:HG13	1:B:823:GLY:H	1.49	0.76
1:B:618:THR:HB	1:B:625:GLN:HG3	1.65	0.76
1:B:819:ALA:CA	1:B:822:ILE:HG21	2.14	0.76
1:B:743:SER:HA	1:B:762:ARG:CZ	2.15	0.76
1:B:822:ILE:HG13	1:B:823:GLY:N	2.00	0.76
1:B:860:THR:O	1:B:863:THR:HG22	1.85	0.76
1:A:562:LEU:O	1:A:562:LEU:CD2	2.30	0.76
1:B:520:HIS:ND1	1:B:525:ARG:HB3	2.01	0.76
1:B:654:LEU:HD11	1:B:674:VAL:HG13	1.66	0.76
1:B:65:LEU:HD21	1:B:80:TRP:CE3	2.20	0.76
1:B:693:MET:SD	1:B:731:TYR:CZ	2.78	0.76
1:B:1:MET:HB3	1:B:2:GLU:C	2.06	0.75
1:B:649:ALA:C	1:B:650:PHE:CD2	2.60	0.75
1:A:720:ILE:CG2	1:A:724:ILE:CD1	2.64	0.75
1:B:683:SER:O	1:B:685:ILE:HD13	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ALA:CA	1:B:650:PHE:CD2	2.70	0.75
1:B:634:THR:O	1:B:638:VAL:CG2	2.34	0.75
1:B:592:LEU:HD12	1:B:638:VAL:HG11	1.68	0.75
1:A:870:ARG:HG3	1:B:342:TRP:HB3	1.69	0.75
1:B:128:GLU:O	1:B:132:GLN:HB2	1.87	0.75
2:C:34:LYS:O	2:C:35:TYR:CB	2.33	0.74
1:A:720:ILE:HG23	1:A:724:ILE:CD1	2.16	0.74
1:B:515:ASP:HB2	1:B:557:ARG:CZ	2.16	0.74
1:A:411:PRO:HG3	1:A:448:TYR:CE1	2.21	0.74
1:B:644:LEU:HD13	1:B:684:ASN:ND2	2.01	0.74
1:B:560:GLN:HG2	1:B:564:MET:CE	2.17	0.74
1:B:649:ALA:HA	1:B:650:PHE:CE2	2.22	0.74
1:B:685:ILE:H	1:B:685:ILE:CD1	2.01	0.74
1:A:37:LEU:CD2	1:A:61:ILE:HD13	2.18	0.73
1:A:720:ILE:CG2	1:A:724:ILE:HD11	2.18	0.73
1:B:686:ILE:HG13	1:B:687:PRO:HD3	0.73	0.73
1:A:561:VAL:CA	1:A:564:MET:HG3	2.13	0.73
1:B:823:GLY:HA2	1:B:824:ASP:O	1.88	0.73
1:B:618:THR:HG22	1:B:622:GLY:HA3	1.70	0.73
1:B:686:ILE:HG12	1:B:687:PRO:HD2	1.69	0.73
1:B:626:GLU:C	1:B:628:ALA:H	1.91	0.73
1:B:801:ILE:HD12	1:B:818:ALA:HA	1.69	0.73
1:B:801:ILE:HD12	1:B:818:ALA:CB	2.19	0.73
1:A:3:LEU:HD22	1:A:6:ILE:HD11	1.70	0.73
1:B:787:VAL:CB	1:B:789:LEU:HD11	2.19	0.72
1:A:784:HIS:N	1:A:785:PRO:CD	2.53	0.72
1:A:798:LEU:HA	1:A:801:ILE:HG12	1.69	0.72
1:A:798:LEU:HD23	1:A:801:ILE:HD11	1.71	0.72
1:B:3:LEU:O	1:B:6:ILE:CG2	2.32	0.72
1:B:592:LEU:HD13	1:B:638:VAL:CG1	2.19	0.72
1:B:721:ALA:CA	1:B:724:ILE:HG22	2.16	0.72
1:A:798:LEU:HA	1:A:801:ILE:CD1	2.20	0.72
1:B:848:THR:CA	1:B:851:ARG:HE	1.97	0.71
1:A:121:ILE:N	1:A:122:PRO:HD2	2.05	0.71
1:B:2:GLU:OE2	1:B:4:ILE:HD13	1.91	0.71
1:A:870:ARG:HH21	1:B:277:LEU:CD2	2.01	0.71
1:B:705:VAL:O	1:B:707:ARG:CB	2.30	0.71
1:B:727:GLU:N	1:B:727:GLU:CD	2.44	0.71
1:A:653:PHE:HA	1:A:656:ILE:HG22	1.73	0.71
1:B:762:ARG:HD2	1:B:800:PHE:CE1	2.24	0.71
1:B:96:LEU:HD21	1:B:132:GLN:CG	2.13	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:LEU:O	1:A:829:PHE:HB2	1.91	0.71
1:B:825:LEU:HD23	1:B:825:LEU:H	1.54	0.71
1:A:864:TRP:CH2	2:C:63:ARG:HD2	2.25	0.70
1:B:105:ARG:HB2	1:B:106:PRO:CD	2.21	0.70
1:A:867:LYS:NZ	1:B:341:ASP:OD2	2.23	0.70
1:B:641:GLY:C	1:B:642:GLU:HG3	2.09	0.70
1:A:856:ASN:O	1:A:857:LYS:HG2	1.92	0.70
1:B:46:ASN:HB3	1:B:49:ASN:HB2	1.74	0.70
1:B:681:LEU:CD1	1:B:685:ILE:HG22	2.01	0.70
1:A:870:ARG:CZ	1:B:342:TRP:CD1	2.66	0.69
1:B:1:MET:HB2	1:B:3:LEU:CD2	2.21	0.69
1:B:759:ASN:ND2	1:B:814:VAL:CA	2.50	0.69
1:A:535:ILE:HD13	1:A:535:ILE:O	1.92	0.69
1:A:117:ALA:HA	1:A:121:ILE:HD13	1.72	0.69
1:B:626:GLU:OE1	1:B:626:GLU:HA	1.92	0.69
1:B:819:ALA:O	1:B:822:ILE:HD13	1.91	0.69
1:A:870:ARG:CG	1:B:342:TRP:HB3	2.22	0.69
1:A:841:PRO:HB2	1:B:232:ARG:NH1	2.07	0.69
1:B:235:VAL:HG21	1:B:274:GLU:HG3	1.75	0.69
1:A:782:ASN:CA	1:B:574:ARG:HB2	2.21	0.69
1:B:561:VAL:HA	1:B:564:MET:SD	2.33	0.69
1:B:801:ILE:HG23	1:B:818:ALA:HB1	1.75	0.69
1:B:819:ALA:C	1:B:822:ILE:HG21	2.13	0.69
1:B:9:LYS:HD2	1:B:17:GLU:OE1	1.93	0.69
1:A:105:ARG:HB2	1:A:106:PRO:HD3	1.74	0.68
1:A:870:ARG:NH2	1:B:277:LEU:HD13	2.07	0.68
1:B:410:MET:O	1:B:414:ILE:HG12	1.93	0.68
1:B:818:ALA:C	1:B:820:GLY:H	1.97	0.68
1:B:364:VAL:N	1:B:365:PRO:HD2	2.09	0.68
1:B:560:GLN:O	1:B:564:MET:HG3	1.92	0.68
1:B:136:ASN:HB3	1:B:146:MET:HE2	1.75	0.68
1:B:766:LEU:HD22	1:B:797:ILE:CG2	2.24	0.68
1:B:11:VAL:CG2	1:B:52:VAL:HG11	2.22	0.68
1:B:821:LEU:O	1:B:821:LEU:CD1	2.37	0.68
1:A:130:ILE:CD1	1:A:169:LYS:HB3	2.23	0.67
1:B:121:ILE:HD11	1:B:129:LEU:HD23	1.75	0.67
1:B:801:ILE:CD1	1:B:818:ALA:HA	2.24	0.67
1:A:179:GLN:HE21	1:A:179:GLN:HA	1.60	0.67
1:B:46:ASN:O	1:B:49:ASN:CB	2.42	0.67
1:B:630:MET:HG2	1:B:669:ALA:HB1	1.76	0.67
1:A:561:VAL:HG22	1:A:564:MET:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:LYS:HB2	1:A:787:VAL:HG11	1.75	0.67
1:B:395:GLU:O	1:B:397:PRO:CD	2.42	0.67
1:B:834:LEU:HD21	1:B:873:LYS:HG2	1.75	0.67
1:A:397:PRO:HB2	1:A:402:LEU:HD11	1.76	0.67
1:B:679:ARG:NH1	1:B:679:ARG:HG3	2.08	0.67
1:B:826:CYS:SG	1:B:865:ALA:O	2.52	0.67
1:A:798:LEU:HA	1:A:801:ILE:CG1	2.24	0.67
1:B:69:ASP:HB2	1:B:72:ILE:HG22	1.71	0.67
1:B:1:MET:CB	1:B:3:LEU:CD2	2.72	0.67
1:B:3:LEU:HD11	1:B:24:PHE:HZ	1.53	0.67
1:B:840:ARG:HB3	1:B:843:ILE:CD1	2.24	0.67
1:B:105:ARG:CB	1:B:106:PRO:CD	2.72	0.67
1:B:94:TYR:O	1:B:97:GLN:HB2	1.95	0.67
1:A:783:VAL:H	1:B:574:ARG:CB	2.09	0.66
1:B:676:ASP:O	1:B:679:ARG:HG2	1.96	0.66
1:B:1:MET:CG	1:B:3:LEU:HD21	2.25	0.66
1:B:631:ALA:O	1:B:635:LEU:HD22	1.94	0.66
1:B:671:VAL:CG1	1:B:709:VAL:HG13	2.25	0.66
1:B:71:ASP:O	1:B:74:ALA:N	2.29	0.66
1:A:782:ASN:N	1:A:782:ASN:HD22	1.94	0.66
1:A:46:ASN:HB3	1:A:49:ASN:ND2	2.10	0.66
1:B:67:SER:HB2	1:B:72:ILE:O	1.95	0.66
1:A:561:VAL:O	1:A:564:MET:HB2	1.95	0.65
1:B:92:LYS:HD3	1:B:120:GLU:OE2	1.95	0.65
1:B:337:ASP:O	1:B:338:ASP:C	2.33	0.65
1:B:654:LEU:HG	1:B:674:VAL:HG22	1.78	0.65
1:B:827:THR:OG1	1:B:864:TRP:HH2	1.76	0.65
1:B:516:ARG:NE	1:B:518:ASP:HB3	2.12	0.65
1:B:46:ASN:O	1:B:49:ASN:HB2	1.96	0.65
1:A:811:THR:HG23	1:A:814:VAL:HG23	1.78	0.65
1:A:783:VAL:H	1:B:574:ARG:HB2	1.61	0.65
1:B:644:LEU:O	1:B:644:LEU:CD1	2.44	0.65
1:B:831:LYS:HB2	1:B:872:LEU:HD12	1.78	0.65
1:A:466:VAL:O	1:A:470:VAL:HG23	1.96	0.64
1:B:464:PRO:HA	1:B:524:LEU:HD12	1.79	0.64
1:B:811:THR:CG2	1:B:814:VAL:CG2	2.75	0.64
1:A:719:ASP:OD2	2:C:55:ARG:NH1	2.31	0.64
1:A:178:ILE:HD12	1:A:217:PHE:HE2	1.63	0.64
1:B:337:ASP:O	1:B:339:ASP:N	2.30	0.64
1:B:377:ASN:ND2	1:B:378:PRO:HD2	2.12	0.64
1:A:360:GLU:CG	1:A:396:GLY:O	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:VAL:O	1:A:636:VAL:HG23	1.98	0.64
1:B:762:ARG:O	1:B:766:LEU:HG	1.98	0.64
1:A:706:HIS:HA	1:A:707:ARG:HB3	1.79	0.64
1:A:734:VAL:O	1:A:737:ASN:HB2	1.98	0.64
1:A:410:MET:HB2	1:A:411:PRO:HD3	1.80	0.64
1:B:854:LYS:N	1:B:854:LYS:HD3	2.13	0.63
1:A:864:TRP:HH2	2:C:63:ARG:HD2	1.62	0.63
1:B:626:GLU:C	1:B:628:ALA:N	2.50	0.63
1:B:6:ILE:HG23	1:B:7:LEU:H	1.62	0.63
1:B:766:LEU:HD22	1:B:797:ILE:HG23	1.80	0.63
1:A:431:THR:O	1:A:435:ILE:HG13	1.98	0.63
1:B:651:LYS:CD	1:B:691:GLU:HB3	2.24	0.63
1:B:3:LEU:C	1:B:6:ILE:HG22	2.16	0.63
1:A:356:ALA:CB	1:A:363:ILE:HD12	2.29	0.63
1:A:720:ILE:HG22	1:A:724:ILE:HD11	1.81	0.63
1:B:453:LEU:HD21	1:B:499:LEU:HD22	1.80	0.63
1:B:831:LYS:CB	1:B:872:LEU:HD12	2.28	0.62
1:A:871:LYS:NZ	1:A:874:ASN:HB2	2.14	0.62
1:A:121:ILE:HD11	1:A:129:LEU:HD22	1.81	0.62
1:A:689:CYS:SG	1:A:724:ILE:HG21	2.39	0.62
1:A:782:ASN:ND2	1:A:782:ASN:N	2.48	0.62
1:A:783:VAL:N	1:B:574:ARG:HB2	2.13	0.62
1:B:785:PRO:N	1:B:786:ASP:HB3	2.14	0.62
1:A:70:PRO:HG2	1:A:754:MET:HG2	1.81	0.62
1:B:36:PHE:CZ	1:B:40:LEU:HD11	2.35	0.62
1:A:691:GLU:O	1:A:694:GLN:HB3	1.98	0.62
1:B:65:LEU:HD13	1:B:116:ILE:HG12	1.81	0.62
1:B:801:ILE:HD12	1:B:818:ALA:CA	2.29	0.62
1:A:798:LEU:CA	1:A:801:ILE:HG12	2.29	0.62
1:B:822:ILE:HD11	1:B:861:LEU:CB	2.25	0.62
1:A:544:TYR:OH	1:A:596:GLN:HG3	2.00	0.62
1:B:74:ALA:O	1:B:78:GLN:HG2	2.00	0.62
1:A:319:LEU:HD11	1:A:363:ILE:HG22	1.82	0.62
1:A:720:ILE:O	1:A:724:ILE:HG12	2.00	0.62
1:A:743:SER:HB2	1:A:796:PHE:HZ	1.65	0.62
1:A:798:LEU:HA	1:A:801:ILE:HD11	1.80	0.62
1:B:811:THR:CG2	1:B:814:VAL:HG23	2.23	0.62
1:A:614:MET:SD	1:A:624:VAL:HB	2.40	0.62
1:B:679:ARG:HH11	1:B:679:ARG:CG	2.04	0.62
1:A:608:MET:HE3	1:A:632:VAL:HG13	1.80	0.61
1:A:636:VAL:O	1:A:636:VAL:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:MET:SD	1:A:754:MET:N	2.69	0.61
1:B:766:LEU:HD13	1:B:821:LEU:CB	2.29	0.61
1:A:755:VAL:C	1:A:757:TYR:H	2.02	0.61
1:B:859:LYS:O	1:B:859:LYS:HG2	1.99	0.61
1:A:118:CYS:HA	1:A:161:ILE:CD1	2.25	0.61
1:A:356:ALA:CA	1:A:363:ILE:CD1	2.76	0.61
1:B:821:LEU:HA	1:B:824:ASP:HB2	1.83	0.61
1:B:8:GLU:O	1:B:11:VAL:HG22	2.00	0.61
1:B:618:THR:CG2	1:B:622:GLY:HA3	2.30	0.61
1:B:722:LEU:HD11	2:D:62:ALA:HB1	1.78	0.61
1:A:561:VAL:HG22	1:A:564:MET:HE3	1.83	0.61
1:A:867:LYS:NZ	1:B:334:ASP:OD2	2.33	0.61
1:B:560:GLN:HG2	1:B:564:MET:HE3	1.83	0.61
1:A:14:ASP:HB3	1:A:17:GLU:HB3	1.82	0.61
1:A:793:ARG:O	1:A:797:ILE:HG12	2.00	0.61
2:C:39:GLU:HG2	2:C:40:GLN:N	2.15	0.61
1:A:565:GLU:CD	1:A:624:VAL:CG1	2.70	0.60
1:A:710:LYS:N	1:A:711:PRO:HD2	2.16	0.60
1:B:703:GLU:HA	1:B:704:ASN:O	2.01	0.60
1:B:759:ASN:HD22	1:B:814:VAL:CB	2.14	0.60
1:B:762:ARG:HB2	1:B:800:PHE:CZ	2.36	0.60
1:B:836:LEU:O	1:B:840:ARG:NH1	2.33	0.60
1:B:707:ARG:H	1:B:707:ARG:HD3	1.65	0.60
1:A:510:LEU:O	1:A:514:THR:HG23	2.02	0.60
1:B:651:LYS:HD3	1:B:691:GLU:CG	2.31	0.60
1:A:747:VAL:HG21	1:A:754:MET:O	2.02	0.60
1:A:867:LYS:HG3	1:B:341:ASP:CG	2.21	0.60
1:B:167:GLN:HG2	1:B:204:PHE:HB2	1.82	0.60
1:B:123:VAL:HG23	1:B:125:GLN:HB2	1.83	0.60
1:B:96:LEU:CD2	1:B:132:GLN:HG2	2.15	0.60
1:B:825:LEU:CD2	1:B:825:LEU:N	2.62	0.60
1:B:529:TYR:O	1:B:533:MET:HG3	2.02	0.60
1:A:871:LYS:O	1:A:871:LYS:HG3	2.02	0.60
1:B:848:THR:HG23	1:B:851:ARG:NH2	2.10	0.60
1:B:766:LEU:CB	1:B:821:LEU:HD23	2.28	0.60
1:A:565:GLU:OE1	1:A:581:GLN:NE2	2.35	0.59
1:B:625:GLN:O	1:B:629:LEU:HG	2.01	0.59
1:B:626:GLU:O	1:B:628:ALA:N	2.35	0.59
1:A:636:VAL:HG22	1:A:643:PHE:CE1	2.36	0.59
1:B:29:ALA:O	1:B:33:LEU:HB2	2.01	0.59
1:B:645:LYS:O	1:B:645:LYS:HG2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:SER:CB	1:B:72:ILE:O	2.50	0.59
1:A:712:GLN:HE21	1:A:712:GLN:HA	1.67	0.59
1:A:755:VAL:O	1:A:757:TYR:N	2.33	0.59
1:B:581:GLN:HE22	1:B:628:ALA:CB	2.15	0.59
1:B:759:ASN:ND2	1:B:814:VAL:O	2.35	0.59
1:B:820:GLY:N	1:B:822:ILE:HG23	2.17	0.59
1:B:831:LYS:O	1:B:834:LEU:CB	2.51	0.59
1:A:181:MET:SD	1:A:195:THR:HA	2.43	0.59
1:A:706:HIS:HD2	1:A:706:HIS:O	1.85	0.59
1:B:689:CYS:O	1:B:693:MET:HB2	2.03	0.59
1:A:22:GLN:O	1:A:26:GLU:HB2	2.03	0.59
1:A:560:GLN:O	1:A:564:MET:CG	2.50	0.59
1:A:104:TYR:CE2	1:A:106:PRO:HD2	2.38	0.59
1:A:356:ALA:CA	1:A:363:ILE:HD13	2.30	0.59
1:B:419:ASP:O	1:B:425:ARG:HD3	2.02	0.59
1:B:845:GLU:HA	1:B:848:THR:HB	1.85	0.59
1:A:130:ILE:HG22	1:A:131:PRO:HD2	1.82	0.58
1:B:759:ASN:HB3	1:B:814:VAL:HG22	1.85	0.58
1:A:405:LEU:O	1:A:408:GLN:HG2	2.03	0.58
1:A:690:ASP:OD1	1:A:730:LYS:NZ	2.36	0.58
1:A:811:THR:CG2	1:A:814:VAL:HG23	2.32	0.58
1:A:83:ILE:HG22	1:A:84:ASP:N	2.18	0.58
1:A:871:LYS:CG	1:B:340:ASP:HA	2.32	0.58
1:B:683:SER:O	1:B:685:ILE:CD1	2.50	0.58
1:B:94:TYR:O	1:B:97:GLN:N	2.33	0.58
1:B:161:ILE:HG21	1:B:166:LEU:HD12	1.83	0.58
1:B:151:LEU:HD13	1:B:194:ALA:HB2	1.85	0.58
1:B:617:SER:O	1:B:618:THR:HG23	2.03	0.58
1:A:857:LYS:HA	1:A:860:THR:HG23	1.84	0.58
1:A:831:LYS:HE2	1:A:876:ALA:CB	2.31	0.58
1:B:360:GLU:HB3	1:B:396:GLY:O	2.04	0.58
1:B:479:GLU:HG2	1:B:538:ASN:ND2	2.18	0.58
1:B:736:LEU:HD22	1:B:793:ARG:HD2	1.85	0.58
1:B:1:MET:CE	1:B:2:GLU:O	2.51	0.58
1:B:681:LEU:H	1:B:681:LEU:HD12	1.68	0.58
1:A:782:ASN:OD1	1:B:574:ARG:HA	2.04	0.58
1:B:520:HIS:CE1	1:B:525:ARG:HB3	2.39	0.58
1:B:833:VAL:O	1:B:833:VAL:HG12	2.03	0.58
1:A:406:VAL:HG21	1:A:439:LEU:HD12	1.86	0.57
1:A:571:THR:O	1:A:575:ILE:HG12	2.04	0.57
1:A:704:ASN:HB3	1:A:705:VAL:HG22	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:LYS:CG	1:A:778:GLY:H	2.03	0.57
1:B:256:MET:HA	1:B:260:LEU:HB2	1.85	0.57
1:B:360:GLU:CB	1:B:396:GLY:O	2.51	0.57
1:B:685:ILE:HD13	1:B:685:ILE:N	2.08	0.57
1:A:151:LEU:HD13	1:A:194:ALA:HB2	1.87	0.57
1:A:238:LEU:O	1:A:242:VAL:HG23	2.04	0.57
1:B:831:LYS:HD3	1:B:872:LEU:O	2.05	0.57
1:A:589:GLN:CG	1:A:634:THR:HG21	2.33	0.57
1:B:516:ARG:HH22	1:B:524:LEU:CD1	2.15	0.57
1:B:801:ILE:HG21	1:B:846:LEU:CD2	2.32	0.57
1:B:870:ARG:O	1:B:874:ASN:N	2.37	0.57
1:A:799:SER:HB3	1:B:104:TYR:OH	2.05	0.57
1:B:712:GLN:HE21	1:B:712:GLN:CA	2.08	0.57
1:B:818:ALA:C	1:B:820:GLY:N	2.58	0.57
1:A:130:ILE:HD11	1:A:172:GLU:CB	2.35	0.57
1:A:3:LEU:HD13	1:A:6:ILE:HD11	1.86	0.57
1:B:1:MET:HG3	1:B:3:LEU:CD2	2.33	0.57
1:B:615:PHE:CZ	1:B:629:LEU:HD23	2.40	0.57
1:B:88:ARG:HH12	1:B:125:GLN:HG3	1.70	0.56
1:A:804:ILE:O	1:A:810:HIS:NE2	2.37	0.56
1:A:769:TYR:CE1	1:A:797:ILE:HD12	2.40	0.56
1:B:581:GLN:HE22	1:B:628:ALA:HB1	1.70	0.56
1:A:870:ARG:HG2	1:B:342:TRP:O	2.05	0.56
1:B:130:ILE:N	1:B:131:PRO:HD2	2.19	0.56
1:B:758:LEU:O	1:B:760:GLU:N	2.39	0.56
1:B:319:LEU:O	1:B:323:VAL:HG23	2.06	0.56
1:B:560:GLN:HG2	1:B:564:MET:HE2	1.85	0.56
1:B:829:PHE:HB2	1:B:833:VAL:CG2	2.35	0.56
1:B:339:ASP:O	1:B:340:ASP:CB	2.50	0.56
1:B:360:GLU:CA	1:B:396:GLY:O	2.53	0.56
1:B:46:ASN:O	1:B:49:ASN:HB3	2.05	0.56
1:B:693:MET:SD	1:B:731:TYR:CE1	2.98	0.56
1:A:783:VAL:HG22	1:A:784:HIS:H	1.69	0.56
1:B:27:ARG:HH11	1:B:27:ARG:CG	2.15	0.56
1:A:743:SER:HB3	1:A:800:PHE:CD1	2.41	0.56
1:B:331:THR:O	1:B:331:THR:HG22	2.05	0.56
1:B:724:ILE:HG23	1:B:724:ILE:O	2.05	0.56
1:A:368:LEU:N	1:A:369:PRO:HD2	2.20	0.56
1:A:453:LEU:HD21	1:A:499:LEU:HD22	1.88	0.56
1:B:360:GLU:HA	1:B:396:GLY:O	2.06	0.56
1:B:847:LEU:O	1:B:851:ARG:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASP:HB3	1:B:17:GLU:HB3	1.88	0.55
1:B:416:LEU:O	1:B:419:ASP:HB2	2.05	0.55
1:B:62:LYS:O	1:B:66:THR:HG22	2.06	0.55
1:B:2:GLU:OE2	1:B:4:ILE:CD1	2.54	0.55
1:B:464:PRO:HB3	1:B:524:LEU:HD12	1.89	0.55
1:A:782:ASN:CB	1:B:574:ARG:CA	2.80	0.55
1:A:720:ILE:CG2	1:A:724:ILE:HD13	2.30	0.55
1:B:646:TYR:O	1:B:648:GLU:N	2.40	0.55
1:B:759:ASN:ND2	1:B:814:VAL:CG1	2.60	0.55
1:B:173:ILE:O	1:B:177:ILE:HG12	2.07	0.55
1:A:161:ILE:HG13	1:A:162:ASP:H	1.72	0.55
1:A:707:ARG:HG3	1:A:707:ARG:O	2.05	0.55
1:A:565:GLU:OE1	1:A:624:VAL:HG11	2.07	0.55
1:B:121:ILE:N	1:B:122:PRO:HD2	2.21	0.55
1:B:377:ASN:C	1:B:377:ASN:HD22	2.09	0.55
1:B:46:ASN:O	1:B:54:ARG:HD2	2.07	0.55
1:B:7:LEU:HA	1:B:10:THR:HG23	1.87	0.55
1:A:364:VAL:N	1:A:365:PRO:HD2	2.22	0.55
1:A:581:GLN:HE22	1:A:624:VAL:HG12	1.72	0.55
1:B:1:MET:HE2	1:B:2:GLU:O	2.06	0.55
1:B:27:ARG:HG3	1:B:27:ARG:NH1	2.18	0.55
1:B:679:ARG:CG	1:B:679:ARG:NH1	2.66	0.55
1:B:763:GLU:HB2	1:B:817:CYS:HB3	1.87	0.55
1:A:356:ALA:HA	1:A:363:ILE:HD12	1.89	0.55
1:A:791:GLN:N	1:A:792:PRO:HD2	2.21	0.55
1:A:117:ALA:CA	1:A:121:ILE:HD13	2.38	0.54
1:B:363:ILE:CD1	1:B:393:ILE:HG22	2.38	0.54
1:B:129:LEU:O	1:B:132:GLN:HB3	2.08	0.54
1:B:639:LEU:HD13	1:B:643:PHE:HZ	1.72	0.54
1:A:362:ASP:N	1:A:362:ASP:OD1	2.34	0.54
1:B:578:ASN:OD1	1:B:624:VAL:HA	2.07	0.54
1:B:851:ARG:O	1:B:852:ARG:HB2	2.06	0.54
1:A:798:LEU:HD23	1:A:801:ILE:CD1	2.38	0.54
1:B:557:ARG:C	1:B:559:GLN:H	2.10	0.54
1:B:6:ILE:HG23	1:B:7:LEU:N	2.22	0.54
1:A:857:LYS:HA	1:A:860:THR:OG1	2.08	0.54
1:B:831:LYS:O	1:B:834:LEU:HB3	2.07	0.54
1:A:130:ILE:N	1:A:131:PRO:HD2	2.22	0.54
1:B:805:ALA:HA	1:B:810:HIS:NE2	2.23	0.54
1:B:848:THR:CG2	1:B:851:ARG:HH21	2.13	0.54
1:B:395:GLU:C	1:B:397:PRO:CD	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:LEU:HA	1:B:769:TYR:HD2	1.73	0.54
1:B:822:ILE:HG22	1:B:846:LEU:HG	1.89	0.54
1:B:830:GLY:CA	1:B:872:LEU:HG	2.35	0.54
1:A:360:GLU:CB	1:A:396:GLY:O	2.56	0.53
1:A:529:TYR:O	1:A:533:MET:HG3	2.08	0.53
1:B:707:ARG:HD3	1:B:707:ARG:N	2.22	0.53
1:B:831:LYS:HB2	1:B:872:LEU:CD1	2.37	0.53
1:B:833:VAL:HG12	1:B:837:VAL:CG2	2.35	0.53
1:A:169:LYS:O	1:A:173:ILE:HD13	2.08	0.53
1:B:824:ASP:O	1:B:826:CYS:N	2.41	0.53
1:B:852:ARG:O	1:B:854:LYS:HD3	2.09	0.53
1:A:42:ARG:HG2	1:A:94:TYR:CZ	2.43	0.53
1:A:565:GLU:OE1	1:A:624:VAL:CG1	2.57	0.53
1:B:364:VAL:N	1:B:365:PRO:CD	2.71	0.53
1:B:46:ASN:OD1	1:B:47:PRO:HD2	2.09	0.53
1:B:759:ASN:ND2	1:B:817:CYS:HB2	2.24	0.53
1:B:852:ARG:O	1:B:854:LYS:HE2	2.09	0.53
1:B:831:LYS:N	1:B:872:LEU:HD12	2.24	0.53
1:B:819:ALA:O	1:B:822:ILE:HG21	2.09	0.53
1:B:822:ILE:CG1	1:B:823:GLY:N	2.69	0.53
1:A:705:VAL:HG12	1:A:706:HIS:CB	2.34	0.53
1:A:69:ASP:CB	1:A:72:ILE:HD12	2.39	0.53
1:B:5:THR:O	1:B:9:LYS:HG2	2.09	0.53
1:B:766:LEU:CD1	1:B:821:LEU:HB2	2.34	0.53
1:B:644:LEU:HD12	1:B:684:ASN:HD21	1.74	0.53
1:A:36:PHE:CE2	1:A:40:LEU:HD11	2.44	0.52
1:B:618:THR:CB	1:B:625:GLN:HG3	2.37	0.52
1:A:870:ARG:CZ	1:B:277:LEU:HD13	2.38	0.52
1:B:637:GLU:OE2	1:B:676:ASP:HB3	2.10	0.52
1:A:121:ILE:N	1:A:122:PRO:CD	2.73	0.52
1:A:128:GLU:OE1	1:A:128:GLU:N	2.42	0.52
1:A:707:ARG:O	1:A:707:ARG:CG	2.54	0.52
1:B:1:MET:CB	1:B:3:LEU:HD21	2.39	0.52
1:B:647:MET:HA	1:B:649:ALA:HB1	1.81	0.52
1:B:736:LEU:HA	1:B:739:LEU:HB2	1.91	0.52
2:C:50:LEU:O	2:C:54:LYS:HG2	2.10	0.52
1:A:174:LEU:O	1:A:178:ILE:HG12	2.09	0.52
1:A:703:GLU:HG3	1:A:703:GLU:O	2.08	0.52
1:B:44:LEU:HG	1:B:98:THR:OG1	2.10	0.52
1:B:464:PRO:CA	1:B:524:LEU:HD12	2.40	0.52
1:B:707:ARG:O	1:B:757:TYR:OH	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ASP:O	1:B:73:LYS:N	2.43	0.52
1:B:786:ASP:CG	1:B:787:VAL:N	2.63	0.52
1:B:633:SER:OG	1:B:673:LEU:HG	2.10	0.52
1:B:822:ILE:HD12	1:B:862:ALA:HB2	1.91	0.52
1:B:867:LYS:HG2	1:B:871:LYS:HD3	1.91	0.52
1:A:161:ILE:HG13	1:A:162:ASP:N	2.24	0.52
1:A:374:HIS:ND1	1:A:382:TYR:HB3	2.25	0.52
1:A:374:HIS:CE1	1:A:382:TYR:CD2	2.98	0.52
1:A:367:VAL:O	1:A:371:ILE:HG12	2.09	0.51
1:A:687:PRO:HG2	1:A:688:PHE:CE1	2.45	0.51
1:B:859:LYS:O	1:B:863:THR:N	2.33	0.51
1:A:120:GLU:C	1:A:122:PRO:HD2	2.29	0.51
1:A:444:ILE:H	1:A:444:ILE:HD12	1.75	0.51
1:A:559:GLN:O	1:A:561:VAL:N	2.43	0.51
1:A:755:VAL:C	1:A:757:TYR:N	2.63	0.51
1:B:736:LEU:HD13	1:B:793:ARG:CZ	2.40	0.51
1:B:75:GLN:O	1:B:79:ARG:HB2	2.10	0.51
1:B:834:LEU:HD21	1:B:873:LYS:HB3	1.92	0.51
1:B:823:GLY:HA3	1:B:865:ALA:HB2	1.91	0.51
1:A:798:LEU:O	1:A:801:ILE:HG13	2.10	0.51
1:B:46:ASN:C	1:B:49:ASN:HB2	2.31	0.51
1:B:510:LEU:O	1:B:514:THR:HG23	2.10	0.51
1:A:696:LEU:HD22	1:A:713:ILE:HG12	1.93	0.51
1:B:766:LEU:HD22	1:B:797:ILE:HG21	1.93	0.51
1:A:393:ILE:HD12	1:A:393:ILE:O	2.10	0.51
1:B:766:LEU:HD13	1:B:821:LEU:CG	2.40	0.51
1:B:807:ASP:O	1:B:810:HIS:CD2	2.63	0.51
1:B:651:LYS:O	1:B:654:LEU:HB2	2.11	0.51
1:B:683:SER:C	1:B:685:ILE:HD12	2.30	0.51
2:C:60:ASN:HA	2:C:63:ARG:HG3	1.93	0.51
1:A:360:GLU:HA	1:A:396:GLY:O	2.11	0.51
1:A:444:ILE:HD12	1:A:444:ILE:N	2.26	0.51
1:B:173:ILE:CD1	1:B:173:ILE:H	2.24	0.51
1:B:84:ASP:OD2	1:B:86:ASN:HB2	2.11	0.51
1:A:405:LEU:HA	1:A:408:GLN:HG2	1.91	0.51
1:A:130:ILE:HG23	1:A:131:PRO:N	2.20	0.50
1:A:831:LYS:HG2	1:A:831:LYS:O	2.10	0.50
1:B:88:ARG:HH12	1:B:125:GLN:CG	2.23	0.50
1:B:405:LEU:O	1:B:408:GLN:HG2	2.11	0.50
1:A:6:ILE:CD1	1:A:24:PHE:HE1	2.24	0.50
1:A:3:LEU:O	1:A:6:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:LYS:HE2	1:B:691:GLU:CD	2.32	0.50
1:B:563:GLN:HE21	1:B:563:GLN:C	2.14	0.50
1:B:683:SER:C	1:B:685:ILE:CD1	2.80	0.50
1:B:718:GLY:O	1:B:722:LEU:HB2	2.11	0.50
1:A:6:ILE:CD1	1:A:24:PHE:CE1	2.94	0.50
1:A:686:ILE:CA	1:A:689:CYS:SG	2.89	0.50
1:A:856:ASN:C	1:A:857:LYS:CG	2.78	0.50
1:B:791:GLN:N	1:B:792:PRO:HD2	2.26	0.50
1:B:821:LEU:C	1:B:824:ASP:HB2	2.32	0.50
1:A:319:LEU:O	1:A:323:VAL:HG23	2.12	0.50
1:A:502:SER:O	1:A:506:ILE:HG12	2.11	0.50
1:A:654:LEU:O	1:A:658:LEU:HG	2.11	0.50
1:A:685:ILE:CD1	1:A:688:PHE:HB2	2.38	0.50
1:B:72:ILE:O	1:B:72:ILE:HG23	2.11	0.50
1:B:681:LEU:N	1:B:681:LEU:HD12	2.26	0.50
1:B:6:ILE:O	1:B:9:LYS:HB2	2.12	0.50
1:B:800:PHE:C	1:B:800:PHE:CD1	2.85	0.50
1:A:867:LYS:HE3	1:B:341:ASP:HB2	1.93	0.50
1:B:823:GLY:HA3	1:B:826:CYS:HB2	1.94	0.50
1:B:833:VAL:O	1:B:837:VAL:HG23	2.12	0.50
1:A:6:ILE:HD12	1:A:24:PHE:CE1	2.47	0.50
1:A:798:LEU:CD2	1:A:801:ILE:HD11	2.41	0.50
1:A:841:PRO:HB3	1:B:192:LEU:HD23	1.93	0.50
1:B:819:ALA:O	1:B:822:ILE:CG2	2.57	0.50
1:A:328:GLN:O	1:A:331:THR:HB	2.12	0.49
1:A:331:THR:O	1:A:331:THR:HG22	2.12	0.49
1:A:406:VAL:HG21	1:A:439:LEU:CD1	2.42	0.49
1:A:781:GLU:HG2	1:A:782:ASN:O	2.12	0.49
1:A:853:SER:HB2	1:A:859:LYS:HD3	1.94	0.49
1:B:358:CYS:SG	1:B:359:CYS:N	2.67	0.49
1:B:377:ASN:ND2	1:B:378:PRO:N	2.56	0.49
1:B:588:LEU:HA	1:B:591:VAL:HG22	1.93	0.49
1:B:581:GLN:NE2	1:B:628:ALA:CB	2.75	0.49
1:B:649:ALA:C	1:B:650:PHE:CG	2.85	0.49
1:B:738:THR:HG22	1:B:761:LEU:HD21	1.94	0.49
1:A:753:ASP:O	1:A:753:ASP:CG	2.49	0.49
1:A:845:GLU:HG3	1:B:232:ARG:HD3	1.93	0.49
1:B:46:ASN:CB	1:B:49:ASN:HB2	2.41	0.49
1:A:130:ILE:HD11	1:A:172:GLU:HB3	1.92	0.49
1:A:489:ASP:O	1:A:490:ASP:HB2	2.11	0.49
1:A:600:ALA:HB1	1:A:638:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:LEU:C	1:A:801:ILE:HG12	2.32	0.49
1:A:5:THR:O	1:A:9:LYS:HG2	2.11	0.49
1:B:222:VAL:O	1:B:226:THR:HG23	2.12	0.49
1:B:272:ILE:HD12	1:B:272:ILE:N	2.28	0.49
1:A:319:LEU:HD12	1:A:355:LEU:HD22	1.92	0.49
1:A:39:GLU:O	1:A:43:VAL:HG23	2.12	0.49
1:A:783:VAL:HG22	1:A:784:HIS:N	2.27	0.49
1:B:316:LYS:HA	1:B:359:CYS:SG	2.52	0.49
1:B:406:VAL:HG21	1:B:439:LEU:HD12	1.94	0.49
1:B:468:SER:O	1:B:471:CYS:HB2	2.13	0.49
1:B:618:THR:O	1:B:625:GLN:HG3	2.12	0.49
1:A:753:ASP:O	1:A:755:VAL:O	2.30	0.49
1:B:766:LEU:HA	1:B:769:TYR:CD2	2.48	0.49
1:A:753:ASP:OD2	1:A:753:ASP:O	2.30	0.49
1:A:870:ARG:HH21	1:B:277:LEU:HD13	1.78	0.49
1:A:841:PRO:HB3	1:B:192:LEU:CD2	2.43	0.49
1:B:520:HIS:ND1	1:B:525:ARG:CB	2.73	0.49
1:A:202:LEU:HD11	1:A:240:ASN:HD22	1.78	0.49
1:A:411:PRO:HA	1:A:414:ILE:HD12	1.94	0.49
1:A:854:LYS:O	1:A:855:THR:O	2.30	0.49
1:B:181:MET:HE1	1:B:198:LEU:HD22	1.95	0.49
1:A:377:ASN:ND2	1:A:379:ASP:H	2.03	0.49
1:A:706:HIS:CA	1:A:707:ARG:HB3	2.40	0.49
1:B:321:TYR:O	1:B:325:ILE:HG12	2.13	0.49
1:A:736:LEU:O	1:A:740:GLN:HB2	2.13	0.49
1:B:465:ARG:HG2	1:B:522:ASN:ND2	2.27	0.49
1:B:651:LYS:HD3	1:B:691:GLU:CD	2.33	0.49
1:B:73:LYS:HG3	1:B:73:LYS:O	2.12	0.49
1:A:496:THR:HA	1:A:540:ALA:HB1	1.95	0.48
1:B:650:PHE:CD2	1:B:650:PHE:N	2.81	0.48
1:B:651:LYS:HE2	1:B:691:GLU:OE1	2.13	0.48
1:B:867:LYS:O	1:B:871:LYS:HG2	2.12	0.48
1:A:360:GLU:O	1:A:361:ASP:C	2.51	0.48
1:A:425:ARG:NH2	1:A:463:GLU:OE1	2.46	0.48
1:B:363:ILE:HD13	1:B:393:ILE:HG22	1.94	0.48
1:B:736:LEU:HD13	1:B:793:ARG:NE	2.27	0.48
1:B:845:GLU:O	1:B:849:GLU:N	2.37	0.48
1:B:834:LEU:CD2	1:B:873:LYS:HB3	2.43	0.48
1:B:818:ALA:C	1:B:846:LEU:HD11	2.34	0.48
1:A:226:THR:O	1:A:234:ARG:HD3	2.14	0.48
1:A:3:LEU:HD22	1:A:6:ILE:CD1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:GLN:O	1:A:666:VAL:HG13	2.13	0.48
1:B:360:GLU:O	1:B:397:PRO:HG3	2.14	0.48
1:B:651:LYS:O	1:B:654:LEU:CB	2.61	0.48
1:B:69:ASP:CB	1:B:72:ILE:CG2	2.74	0.48
1:B:72:ILE:HG12	1:B:72:ILE:O	2.13	0.48
1:B:775:GLY:C	1:B:780:GLN:N	2.67	0.48
1:A:513:THR:HG23	1:A:516:ARG:HD3	1.95	0.48
1:B:264:THR:HG21	1:B:282:PHE:CE2	2.49	0.48
1:B:740:GLN:O	1:B:743:SER:HB2	2.13	0.48
1:A:161:ILE:HG21	1:A:166:LEU:HD12	1.96	0.48
1:A:177:ILE:HD12	1:A:197:ALA:HB1	1.96	0.48
1:B:377:ASN:C	1:B:377:ASN:ND2	2.66	0.48
1:A:419:ASP:O	1:A:425:ARG:HD3	2.13	0.48
1:A:706:HIS:CG	1:A:706:HIS:O	2.67	0.48
1:A:797:ILE:O	1:A:801:ILE:HG23	2.14	0.48
1:B:1:MET:CG	1:B:3:LEU:CD2	2.91	0.48
1:B:829:PHE:HB2	1:B:833:VAL:HG23	1.96	0.48
2:C:61:HIS:C	2:C:61:HIS:ND1	2.66	0.48
1:A:513:THR:HA	1:A:516:ARG:HG3	1.95	0.48
1:B:707:ARG:CD	1:B:707:ARG:N	2.77	0.48
1:A:682:GLN:HE21	1:A:682:GLN:HB2	1.53	0.47
1:A:356:ALA:CB	1:A:363:ILE:CD1	2.92	0.47
1:A:497:TYR:CD1	1:A:540:ALA:HB2	2.49	0.47
1:A:559:GLN:C	1:A:561:VAL:N	2.66	0.47
1:B:514:THR:HB	1:B:529:TYR:CZ	2.49	0.47
1:B:620:GLY:O	1:B:621:SER:HB2	2.14	0.47
1:B:615:PHE:HA	1:B:625:GLN:HE21	1.79	0.47
1:A:560:GLN:O	1:A:564:MET:HE2	2.14	0.47
1:A:782:ASN:H	1:A:782:ASN:HD22	1.62	0.47
1:B:132:GLN:HE21	1:B:136:ASN:HD21	1.62	0.47
1:A:375:ILE:HD11	1:A:412:THR:HG22	1.97	0.47
1:A:807:ASP:C	1:A:809:ASP:H	2.17	0.47
1:B:851:ARG:O	1:B:852:ARG:CB	2.62	0.47
1:B:686:ILE:N	1:B:687:PRO:HD2	2.30	0.47
1:B:797:ILE:CG2	1:B:821:LEU:HG	2.45	0.47
1:B:393:ILE:O	1:B:393:ILE:HD12	2.15	0.47
1:B:686:ILE:N	1:B:687:PRO:CD	2.77	0.47
1:A:177:ILE:HD12	1:A:197:ALA:CB	2.45	0.47
1:A:782:ASN:HB3	1:B:574:ARG:HA	1.92	0.47
1:A:798:LEU:O	1:A:801:ILE:CG1	2.62	0.47
1:B:130:ILE:CG1	1:B:131:PRO:HD2	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:SER:O	1:B:152:GLU:HB2	2.15	0.47
1:B:19:GLU:HA	1:B:19:GLU:OE2	2.13	0.47
1:B:1:MET:HB2	1:B:3:LEU:HD21	1.93	0.47
1:B:712:GLN:HA	1:B:712:GLN:NE2	2.15	0.47
1:B:824:ASP:C	1:B:826:CYS:H	2.18	0.47
1:B:516:ARG:NH2	1:B:524:LEU:CD1	2.72	0.47
1:B:766:LEU:CD2	1:B:797:ILE:HG23	2.45	0.47
1:B:804:ILE:HD12	1:B:814:VAL:CG1	2.41	0.47
1:B:855:THR:O	1:B:858:ALA:HB3	2.14	0.47
1:B:464:PRO:CB	1:B:524:LEU:HD12	2.45	0.47
1:B:843:ILE:C	1:B:845:GLU:H	2.19	0.47
1:B:859:LYS:O	1:B:863:THR:HB	2.15	0.47
1:A:338:ASP:C	1:A:340:ASP:H	2.18	0.47
1:A:559:GLN:C	1:A:561:VAL:H	2.18	0.47
1:A:712:GLN:NE2	1:A:712:GLN:HA	2.29	0.47
1:B:453:LEU:HD21	1:B:499:LEU:CD2	2.43	0.47
1:B:859:LYS:O	1:B:863:THR:CB	2.63	0.47
1:A:130:ILE:HD11	1:A:172:GLU:HB2	1.97	0.46
1:A:762:ARG:O	1:A:766:LEU:HG	2.15	0.46
1:A:805:ALA:HA	1:A:810:HIS:HE2	1.80	0.46
1:B:649:ALA:O	1:B:651:LYS:N	2.48	0.46
1:B:700:LEU:HD13	1:B:710:LYS:HE3	1.96	0.46
1:B:834:LEU:HG	1:B:873:LYS:HB3	1.97	0.46
1:A:495:ALA:HA	1:A:541:LYS:HE2	1.98	0.46
1:A:682:GLN:O	1:A:683:SER:HB3	2.15	0.46
1:B:843:ILE:C	1:B:845:GLU:N	2.68	0.46
2:C:27:ARG:O	2:C:29:SER:N	2.48	0.46
1:A:380:TRP:HA	1:A:383:ARG:HB3	1.97	0.46
1:A:383:ARG:NH1	1:A:419:ASP:OD2	2.48	0.46
1:B:681:LEU:CD1	1:B:685:ILE:CG2	2.75	0.46
1:B:821:LEU:CA	1:B:824:ASP:HB2	2.44	0.46
1:A:620:GLY:O	1:A:621:SER:HB2	2.16	0.46
1:B:516:ARG:CZ	1:B:518:ASP:HB3	2.46	0.46
1:B:635:LEU:HA	1:B:638:VAL:HB	1.96	0.46
1:A:595:VAL:HG23	1:A:600:ALA:HB2	1.98	0.46
1:B:46:ASN:HA	1:B:47:PRO:HD3	1.60	0.46
1:B:549:LYS:O	1:B:553:VAL:HG23	2.15	0.46
1:B:804:ILE:HA	1:B:804:ILE:HD13	1.88	0.46
1:B:554:ILE:HD13	1:B:587:THR:HG22	1.96	0.46
1:A:388:MET:HE1	2:C:32:LYS:HE3	1.98	0.46
1:A:777:LYS:HB2	1:A:787:VAL:CG1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ASP:N	1:B:362:ASP:OD1	2.49	0.46
1:B:693:MET:HG2	1:B:731:TYR:HH	1.76	0.46
1:B:811:THR:CG2	1:B:814:VAL:HG21	2.45	0.46
1:A:663:GLU:O	1:A:665:GLN:N	2.48	0.46
1:A:856:ASN:H	1:A:856:ASN:ND2	2.14	0.46
1:B:27:ARG:NH1	1:B:27:ARG:CG	2.76	0.46
1:B:706:HIS:HA	1:B:707:ARG:HD2	1.98	0.46
1:B:724:ILE:HG12	1:B:726:GLY:N	2.31	0.46
1:A:681:LEU:HB3	1:A:684:ASN:HB2	1.97	0.45
1:B:33:LEU:HD21	1:B:83:ILE:HD11	1.98	0.45
1:B:511:LEU:O	1:B:557:ARG:NH2	2.46	0.45
1:B:718:GLY:HA3	1:B:768:ALA:HA	1.98	0.45
1:B:831:LYS:O	1:B:834:LEU:HB2	2.15	0.45
2:D:56:LEU:O	2:D:60:ASN:N	2.49	0.45
1:A:305:ARG:HA	1:A:306:PRO:HD3	1.85	0.45
1:A:83:ILE:CG2	1:A:84:ASP:N	2.79	0.45
1:B:573:ASP:HA	1:B:576:GLN:CB	2.37	0.45
1:A:793:ARG:HB3	1:A:797:ILE:HD11	1.98	0.45
1:B:395:GLU:C	1:B:397:PRO:HD2	2.37	0.45
1:B:513:THR:HA	1:B:516:ARG:HD3	1.97	0.45
1:A:117:ALA:O	1:A:121:ILE:HD13	2.16	0.45
1:A:136:ASN:HB3	1:A:146:MET:HE2	1.99	0.45
1:A:755:VAL:HG23	1:A:756:ASP:N	2.03	0.45
1:A:811:THR:O	1:A:813:GLY:N	2.50	0.45
1:B:129:LEU:O	1:B:132:GLN:N	2.48	0.45
1:B:142:SER:HB3	1:B:146:MET:HG2	1.98	0.45
1:B:692:VAL:O	1:B:696:LEU:HG	2.15	0.45
1:B:739:LEU:HD13	1:B:797:ILE:CD1	2.47	0.45
1:A:356:ALA:HA	1:A:363:ILE:HG21	1.99	0.45
1:B:444:ILE:HD12	1:B:498:CYS:SG	2.56	0.45
1:B:518:ASP:C	1:B:518:ASP:OD2	2.55	0.45
1:B:736:LEU:HG	1:B:769:TYR:OH	2.16	0.45
2:D:56:LEU:O	2:D:60:ASN:CB	2.64	0.45
1:A:173:ILE:HD12	1:A:173:ILE:H	1.81	0.45
1:A:659:LYS:HE3	1:A:659:LYS:HB2	1.73	0.45
1:A:759:ASN:HB3	1:A:811:THR:CG2	2.47	0.45
1:B:456:LEU:HB3	1:B:474:PHE:CE2	2.51	0.45
1:B:573:ASP:O	1:B:576:GLN:HB3	2.17	0.45
1:B:684:ASN:ND2	1:B:684:ASN:O	2.49	0.45
1:A:338:ASP:O	1:A:346:LYS:NZ	2.50	0.45
1:A:682:GLN:H	1:A:682:GLN:HG3	1.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:TYR:N	1:B:545:PRO:HD2	2.32	0.45
1:B:581:GLN:NE2	1:B:628:ALA:HB2	2.31	0.45
1:A:356:ALA:CA	1:A:363:ILE:HD12	2.46	0.45
1:A:770:THR:OG1	1:A:821:LEU:HD23	2.17	0.45
1:A:797:ILE:O	1:A:801:ILE:HG12	2.16	0.45
1:B:644:LEU:CB	1:B:684:ASN:OD1	2.53	0.45
1:B:151:LEU:HD12	1:B:190:VAL:HG13	1.98	0.45
1:B:337:ASP:OD2	1:B:465:ARG:HB3	2.17	0.45
1:B:396:GLY:N	1:B:397:PRO:CD	2.80	0.45
1:B:787:VAL:CB	1:B:789:LEU:CD1	2.81	0.45
2:D:57:ASP:O	2:D:60:ASN:N	2.50	0.45
1:A:272:ILE:HD12	1:A:272:ILE:N	2.32	0.45
1:A:331:THR:HG21	1:A:382:TYR:CZ	2.52	0.45
1:A:185:GLU:HA	1:A:186:PRO:HD3	1.76	0.44
1:A:331:THR:O	1:A:331:THR:CG2	2.64	0.44
1:A:787:VAL:C	1:A:789:LEU:H	2.20	0.44
1:A:871:LYS:HG2	1:B:340:ASP:CA	2.39	0.44
1:B:128:GLU:O	1:B:132:GLN:CB	2.60	0.44
1:B:643:PHE:O	1:B:645:LYS:N	2.48	0.44
1:A:374:HIS:HB3	1:A:382:TYR:O	2.17	0.44
1:A:486:ASP:CG	1:A:486:ASP:O	2.56	0.44
1:A:857:LYS:HB3	1:A:860:THR:OG1	2.17	0.44
1:B:120:GLU:HB3	1:B:125:GLN:HB3	2.00	0.44
1:B:136:ASN:HB3	1:B:146:MET:CE	2.46	0.44
1:B:223:CYS:O	1:B:226:THR:OG1	2.30	0.44
1:B:826:CYS:SG	1:B:865:ALA:C	2.95	0.44
1:B:178:ILE:HD13	1:B:181:MET:HE1	1.99	0.44
1:B:801:ILE:HD12	1:B:818:ALA:HB2	1.96	0.44
1:A:343:ASN:HD22	1:A:345:CYS:H	1.66	0.44
1:A:479:GLU:HG2	1:A:538:ASN:ND2	2.31	0.44
1:B:649:ALA:O	1:B:650:PHE:C	2.56	0.44
1:B:95:VAL:C	1:B:97:GLN:H	2.21	0.44
1:A:731:TYR:O	1:A:733:GLU:N	2.51	0.44
1:A:753:ASP:HA	1:A:755:VAL:HG13	1.99	0.44
1:B:859:LYS:O	1:B:863:THR:HG22	2.17	0.44
1:A:105:ARG:CB	1:A:106:PRO:HD3	2.45	0.44
1:A:360:GLU:O	1:A:363:ILE:HG12	2.17	0.44
1:A:498:CYS:O	1:A:499:LEU:CD2	2.58	0.44
1:B:185:GLU:HA	1:B:186:PRO:HD3	1.86	0.44
1:B:724:ILE:CG1	1:B:726:GLY:H	2.30	0.44
1:B:797:ILE:HG22	1:B:821:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:TYR:CZ	1:A:596:GLN:HG3	2.52	0.44
1:A:704:ASN:CB	1:A:705:VAL:CG2	2.77	0.44
1:A:811:THR:CG2	1:A:814:VAL:CG2	2.95	0.44
1:B:502:SER:O	1:B:506:ILE:HG12	2.18	0.44
1:B:670:ALA:O	1:B:674:VAL:HG23	2.18	0.44
1:B:683:SER:CA	1:B:685:ILE:HD12	2.48	0.44
1:B:833:VAL:O	1:B:833:VAL:CG1	2.66	0.44
2:C:49:GLU:HG3	2:C:50:LEU:N	2.32	0.44
1:B:650:PHE:HA	1:B:652:PRO:HD2	2.00	0.44
1:B:173:ILE:CD1	1:B:173:ILE:N	2.81	0.44
1:B:676:ASP:O	1:B:679:ARG:N	2.34	0.44
1:B:759:ASN:ND2	1:B:814:VAL:C	2.72	0.44
1:B:801:ILE:HG21	1:B:846:LEU:HD13	2.00	0.44
2:C:55:ARG:O	2:C:59:VAL:HG23	2.18	0.44
1:A:133:LEU:HD22	1:A:150:THR:HG23	2.00	0.43
1:A:167:GLN:HG2	1:A:204:PHE:HB2	1.98	0.43
1:A:635:LEU:HA	1:A:635:LEU:HD12	1.81	0.43
1:B:670:ALA:O	1:B:673:LEU:N	2.51	0.43
1:B:787:VAL:C	1:B:789:LEU:HG	2.38	0.43
1:A:628:ALA:O	1:A:632:VAL:HG23	2.17	0.43
1:A:712:GLN:CA	1:A:712:GLN:HE21	2.28	0.43
1:A:737:ASN:ND2	1:B:13:PRO:CA	2.57	0.43
1:B:33:LEU:HB3	1:B:34:PRO:HD3	2.00	0.43
1:B:725:GLY:HA2	1:B:726:GLY:O	2.18	0.43
1:B:819:ALA:N	1:B:846:LEU:HD11	2.33	0.43
1:A:360:GLU:O	1:A:362:ASP:N	2.52	0.43
1:A:413:LEU:HA	1:A:416:LEU:HD12	2.01	0.43
1:B:711:PRO:CD	1:B:757:TYR:OH	2.60	0.43
1:B:831:LYS:HB2	1:B:872:LEU:HB3	2.00	0.43
1:B:863:THR:HG23	1:B:864:TRP:N	2.34	0.43
1:A:375:ILE:CD1	1:A:375:ILE:O	2.54	0.43
1:A:706:HIS:CD2	1:A:706:HIS:C	2.89	0.43
1:B:707:ARG:C	1:B:709:VAL:N	2.70	0.43
1:B:834:LEU:HD21	1:B:873:LYS:CG	2.47	0.43
1:A:375:ILE:HD13	1:A:375:ILE:C	2.37	0.43
1:A:403:LYS:N	1:A:404:PRO:HD2	2.33	0.43
1:A:871:LYS:HZ3	1:A:874:ASN:HB2	1.82	0.43
1:B:773:VAL:C	1:B:775:GLY:H	2.22	0.43
1:B:94:TYR:O	1:B:97:GLN:CB	2.65	0.43
1:A:561:VAL:HA	1:A:564:MET:HE2	1.99	0.43
1:A:565:GLU:CD	1:A:624:VAL:HG11	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:GLU:C	1:A:665:GLN:H	2.22	0.43
1:B:371:ILE:CD1	1:B:389:ALA:HB3	2.48	0.43
1:A:783:VAL:N	1:B:574:ARG:CB	2.75	0.43
1:B:636:VAL:O	1:B:636:VAL:HG13	2.19	0.43
1:A:178:ILE:CD1	1:A:217:PHE:HE2	2.31	0.43
1:A:321:TYR:O	1:A:325:ILE:HG12	2.18	0.43
1:A:69:ASP:HB3	1:A:72:ILE:HD12	2.00	0.43
1:A:802:ASP:HA	1:A:843:ILE:HD11	2.00	0.43
1:B:444:ILE:O	1:B:444:ILE:HG22	2.18	0.43
1:B:3:LEU:CB	1:B:6:ILE:CG2	2.80	0.43
1:B:73:LYS:O	1:B:77:GLN:HG3	2.19	0.43
1:B:768:ALA:O	1:B:769:TYR:C	2.57	0.43
1:A:411:PRO:O	1:A:415:GLU:HG3	2.18	0.43
1:A:42:ARG:NH1	1:A:94:TYR:OH	2.51	0.43
1:A:578:ASN:HD22	1:A:578:ASN:HA	1.69	0.43
1:A:759:ASN:HB3	1:A:811:THR:HG21	2.00	0.43
1:B:615:PHE:HB3	1:B:653:PHE:CD1	2.54	0.43
1:B:671:VAL:HG11	1:B:709:VAL:CG1	2.40	0.43
1:B:786:ASP:CG	1:B:787:VAL:H	2.22	0.43
1:A:731:TYR:C	1:A:733:GLU:N	2.72	0.42
1:A:770:THR:HG23	1:A:824:ASP:OD2	2.19	0.42
1:B:135:ALA:O	1:B:139:ASN:HB2	2.19	0.42
1:B:654:LEU:HD12	1:B:677:LEU:HD13	2.01	0.42
1:B:821:LEU:HD22	1:B:824:ASP:HB2	2.01	0.42
1:A:154:ILE:H	1:A:154:ILE:HG13	1.59	0.42
1:A:841:PRO:HB2	1:B:232:ARG:HH11	1.81	0.42
1:B:361:ASP:OD1	1:B:401:GLN:NE2	2.53	0.42
1:B:697:LEU:HD11	1:B:730:LYS:HE3	2.01	0.42
1:B:76:TYR:CD1	1:B:76:TYR:N	2.85	0.42
1:A:388:MET:CE	2:C:32:LYS:HE3	2.49	0.42
1:A:127:PRO:HG2	1:A:128:GLU:OE1	2.19	0.42
1:A:178:ILE:HA	1:A:181:MET:HE2	2.00	0.42
1:A:312:LYS:O	1:A:313:PHE:C	2.57	0.42
1:A:636:VAL:HG22	1:A:643:PHE:CD1	2.53	0.42
1:A:654:LEU:HD23	1:A:654:LEU:HA	1.80	0.42
1:A:728:PHE:O	1:A:729:LYS:C	2.57	0.42
1:A:121:ILE:CD1	1:A:121:ILE:N	2.81	0.42
1:A:150:THR:O	1:A:154:ILE:HG13	2.19	0.42
1:A:402:LEU:O	1:A:406:VAL:HG23	2.19	0.42
1:B:388:MET:HB2	1:B:427:THR:HG21	2.02	0.42
1:B:3:LEU:CA	1:B:6:ILE:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:SER:O	1:B:711:PRO:HG2	2.19	0.42
1:B:714:LEU:HA	1:B:717:PHE:CD2	2.53	0.42
1:A:289:GLU:O	1:A:293:LEU:HG	2.20	0.42
1:A:364:VAL:HB	1:A:365:PRO:CD	2.49	0.42
1:B:683:SER:O	1:B:685:ILE:N	2.50	0.42
1:B:834:LEU:CG	1:B:873:LYS:HB3	2.50	0.42
2:C:39:GLU:HG2	2:C:40:GLN:H	1.83	0.42
1:B:71:ASP:C	1:B:73:LYS:H	2.23	0.42
1:A:518:ASP:OD1	1:A:518:ASP:N	2.52	0.42
1:B:126:TRP:CG	1:B:129:LEU:HB2	2.55	0.42
1:B:636:VAL:O	1:B:636:VAL:CG1	2.67	0.42
1:A:214:GLU:O	1:A:218:ILE:HG12	2.20	0.42
1:A:557:ARG:C	1:A:559:GLN:H	2.23	0.42
1:B:117:ALA:C	1:B:119:ALA:H	2.23	0.42
1:B:407:ILE:HD11	1:B:442:ALA:HA	2.00	0.42
1:B:331:THR:O	1:B:331:THR:CG2	2.67	0.42
1:A:173:ILE:N	1:A:173:ILE:HD12	2.35	0.42
1:A:3:LEU:HA	1:A:6:ILE:CG1	2.49	0.42
1:B:173:ILE:HD12	1:B:173:ILE:N	2.35	0.42
1:B:235:VAL:HG21	1:B:274:GLU:CG	2.47	0.42
1:A:153:ALA:O	1:A:157:ILE:HG13	2.20	0.41
1:A:209:PHE:C	1:A:211:LYS:H	2.23	0.41
1:B:626:GLU:HB3	1:B:627:ASP:H	1.57	0.41
1:A:11:VAL:HG12	1:A:11:VAL:O	2.19	0.41
1:A:375:ILE:HD11	1:A:416:LEU:HD11	2.01	0.41
1:A:426:ASP:OD1	1:A:426:ASP:C	2.58	0.41
1:A:565:GLU:CD	1:A:624:VAL:HG13	2.39	0.41
1:A:68:LYS:N	1:A:68:LYS:HE3	2.35	0.41
1:B:740:GLN:NE2	1:B:744:GLN:OE1	2.53	0.41
1:B:787:VAL:O	1:B:789:LEU:HG	2.20	0.41
1:B:801:ILE:CG2	1:B:846:LEU:HD13	2.50	0.41
1:A:544:TYR:O	1:A:547:VAL:N	2.51	0.41
1:B:235:VAL:O	1:B:239:GLN:HG3	2.21	0.41
1:B:543:CYS:O	1:B:547:VAL:HG23	2.21	0.41
1:B:852:ARG:CG	1:B:852:ARG:HH11	2.12	0.41
1:B:853:SER:C	1:B:854:LYS:HD3	2.40	0.41
1:A:557:ARG:O	1:A:561:VAL:HG23	2.20	0.41
1:B:465:ARG:HG2	1:B:522:ASN:HD21	1.85	0.41
1:B:69:ASP:CB	1:B:72:ILE:HG22	2.46	0.41
1:B:763:GLU:HA	1:B:766:LEU:CD1	2.51	0.41
1:B:788:MET:HE1	1:B:791:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ALA:C	1:A:303:GLN:H	2.22	0.41
1:B:489:ASP:O	1:B:490:ASP:HB2	2.20	0.41
1:B:65:LEU:HD13	1:B:116:ILE:CG1	2.48	0.41
1:B:702:ASN:O	1:B:703:GLU:C	2.59	0.41
1:B:710:LYS:N	1:B:711:PRO:HD2	2.34	0.41
1:A:410:MET:O	1:A:414:ILE:HG13	2.20	0.41
1:A:415:GLU:C	1:A:417:MET:N	2.74	0.41
1:A:383:ARG:NH1	1:A:424:VAL:HG21	2.35	0.41
1:A:622:GLY:HA3	1:A:625:GLN:HB2	2.03	0.41
1:A:677:LEU:HA	1:A:677:LEU:HD23	1.94	0.41
1:B:730:LYS:HB3	1:B:731:TYR:CD1	2.55	0.41
1:B:841:PRO:C	1:B:843:ILE:H	2.23	0.41
1:A:3:LEU:CD2	1:A:6:ILE:HD11	2.48	0.41
1:B:364:VAL:HB	1:B:365:PRO:HD3	2.03	0.41
1:B:644:LEU:O	1:B:644:LEU:CG	2.69	0.41
1:A:397:PRO:HB2	1:A:402:LEU:CD1	2.47	0.41
1:B:149:SER:HA	1:B:152:GLU:HB2	2.03	0.41
1:B:264:THR:HG21	1:B:282:PHE:CD2	2.55	0.41
1:B:626:GLU:OE1	1:B:666:VAL:HG22	2.21	0.41
1:B:680:ALA:HB1	1:B:681:LEU:HD12	2.01	0.41
1:B:738:THR:O	1:B:742:ALA:CB	2.68	0.41
1:B:83:ILE:O	1:B:84:ASP:C	2.58	0.41
1:A:497:TYR:H	1:A:497:TYR:HD1	1.69	0.41
1:A:655:GLY:HA2	1:A:658:LEU:HD12	2.02	0.41
1:B:637:GLU:OE1	1:B:679:ARG:HG3	2.20	0.41
1:B:798:LEU:HB3	1:B:843:ILE:HG13	2.03	0.41
1:A:530:GLU:HA	1:A:533:MET:CE	2.51	0.40
1:A:585:CYS:SG	1:A:631:ALA:HB2	2.62	0.40
1:A:710:LYS:HB3	1:A:711:PRO:CD	2.51	0.40
1:A:867:LYS:CE	1:B:341:ASP:CG	2.89	0.40
1:B:773:VAL:C	1:B:775:GLY:N	2.75	0.40
1:B:818:ALA:O	1:B:820:GLY:N	2.54	0.40
1:A:602:GLN:O	1:A:606:VAL:HG23	2.21	0.40
1:A:710:LYS:N	1:A:711:PRO:CD	2.83	0.40
1:B:625:GLN:O	1:B:629:LEU:CD1	2.69	0.40
1:B:673:LEU:O	1:B:676:ASP:HB2	2.20	0.40
1:B:739:LEU:HD13	1:B:797:ILE:HD11	2.03	0.40
1:A:415:GLU:O	1:A:417:MET:N	2.55	0.40
1:A:450:ALA:N	1:A:451:PRO:HD2	2.37	0.40
1:A:592:LEU:C	1:A:594:LYS:H	2.23	0.40
1:A:709:VAL:O	1:A:710:LYS:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:VAL:C	1:A:789:LEU:N	2.74	0.40
1:B:685:ILE:CD1	1:B:685:ILE:N	2.72	0.40
1:B:697:LEU:CD1	1:B:730:LYS:HE3	2.52	0.40
1:B:763:GLU:HA	1:B:766:LEU:HD12	2.03	0.40
1:B:80:TRP:O	1:B:88:ARG:HD3	2.20	0.40
1:A:3:LEU:C	1:A:6:ILE:HG12	2.41	0.40
1:A:714:LEU:HD22	1:A:739:LEU:HD23	2.02	0.40
1:A:758:LEU:O	1:A:762:ARG:HG3	2.22	0.40
1:A:181:MET:HE1	1:A:198:LEU:HD22	2.04	0.40
1:A:811:THR:HG23	1:A:814:VAL:CG2	2.48	0.40
1:B:178:ILE:HG21	1:B:217:PHE:CZ	2.57	0.40
1:B:368:LEU:N	1:B:369:PRO:HD2	2.37	0.40
1:B:824:ASP:C	1:B:826:CYS:N	2.75	0.40
1:B:826:CYS:SG	1:B:865:ALA:CB	3.09	0.40
1:B:859:LYS:HG2	1:B:863:THR:HB	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	867/876 (99%)	761 (88%)	97 (11%)	9 (1%)	18	61
1	B	834/876 (95%)	712 (85%)	110 (13%)	12 (1%)	13	53
2	C	32/40 (80%)	27 (84%)	4 (12%)	1 (3%)	5	31
2	D	21/40 (52%)	16 (76%)	5 (24%)	0	100	100
All	All	1754/1832 (96%)	1516 (86%)	216 (12%)	22 (1%)	14	55

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	441	GLU
1	A	560	GLN
1	A	732	LEU
1	B	47	PRO
1	B	72	ILE
1	B	627	ASP
1	B	708	SER
1	A	462	ALA
1	A	756	ASP
1	A	808	GLU
1	A	165	GLN
1	A	638	VAL
2	C	28	LEU
1	B	4	ILE
1	B	515	ASP
1	B	677	LEU
1	B	819	ALA
1	B	96	LEU
1	B	687	PRO
1	B	822	ILE
1	A	755	VAL
1	B	157	ILE

### 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	746/751 (99%)	695 (93%)	51 (7%)	18	56
1	B	722/751 (96%)	648 (90%)	74 (10%)	8	34
2	C	35/39 (90%)	31 (89%)	4 (11%)	7	28
All	All	1503/1541 (98%)	1374 (91%)	129 (9%)	12	43

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU

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Mol	Chain	Res	Type
1	A	9	LYS
1	A	32	ASN
1	A	68	LYS
1	A	121	ILE
1	A	128	GLU
1	A	161	ILE
1	A	166	LEU
1	A	175	THR
1	A	179	GLN
1	A	234	ARG
1	A	352	LEU
1	A	362	ASP
1	A	375	ILE
1	A	377	ASN
1	A	408	GLN
1	A	417	MET
1	A	426	ASP
1	A	474	PHE
1	A	497	TYR
1	A	524	LEU
1	A	532	LEU
1	A	535	ILE
1	A	559	GLN
1	A	563	GLN
1	A	580	LEU
1	A	624	VAL
1	A	626	GLU
1	A	634	THR
1	A	635	LEU
1	A	637	GLU
1	A	654	LEU
1	A	673	LEU
1	A	681	LEU
1	A	682	GLN
1	A	685	ILE
1	A	691	GLU
1	A	702	ASN
1	A	703	GLU
1	A	705	VAL
1	A	707	ARG
1	A	708	SER
1	A	753	ASP

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Mol	Chain	Res	Type
1	A	754	MET
1	A	755	VAL
1	A	756	ASP
1	A	781	GLU
1	A	782	ASN
1	A	855	THR
1	A	856	ASN
1	A	857	LYS
2	C	29	SER
2	C	35	TYR
2	C	40	GLN
2	C	61	HIS
1	B	5	THR
1	B	7	LEU
1	B	15	ARG
1	B	71	ASP
1	B	73	LYS
1	B	79	ARG
1	B	146	MET
1	B	166	LEU
1	B	172	GLU
1	B	173	ILE
1	B	213	SER
1	B	234	ARG
1	B	336	ASN
1	B	352	LEU
1	B	362	ASP
1	B	377	ASN
1	B	378	PRO
1	B	400	SER
1	B	417	MET
1	B	465	ARG
1	B	474	PHE
1	B	497	TYR
1	B	532	LEU
1	B	559	GLN
1	B	563	GLN
1	B	580	LEU
1	B	599	ASP
1	B	618	THR
1	B	624	VAL
1	B	625	GLN

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Mol	Chain	Res	Type
1	B	626	GLU
1	B	633	SER
1	B	634	THR
1	B	635	LEU
1	B	636	VAL
1	B	642	GLU
1	B	645	LYS
1	B	647	MET
1	B	650	PHE
1	B	651	LYS
1	B	665	GLN
1	B	673	LEU
1	B	681	LEU
1	B	685	ILE
1	B	689	CYS
1	B	700	LEU
1	B	704	ASN
1	B	706	HIS
1	B	707	ARG
1	B	712	GLN
1	B	722	LEU
1	B	727	GLU
1	B	729	LYS
1	B	731	TYR
1	B	747	VAL
1	B	757	TYR
1	B	758	LEU
1	B	780	GLN
1	B	786	ASP
1	B	787	VAL
1	B	800	PHE
1	B	804	ILE
1	B	807	ASP
1	B	811	THR
1	B	825	LEU
1	B	829	PHE
1	B	834	LEU
1	B	851	ARG
1	B	852	ARG
1	B	853	SER
1	B	854	LYS
1	B	859	LYS

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Mol	Chain	Res	Type
1	B	872	LEU
1	B	873	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	141	ASN
1	A	179	GLN
1	A	208	ASN
1	A	240	ASN
1	A	309	HIS
1	A	320	GLN
1	A	343	ASN
1	A	377	ASN
1	A	401	GLN
1	A	408	GLN
1	A	454	GLN
1	A	521	GLN
1	A	538	ASN
1	A	559	GLN
1	A	578	ASN
1	A	581	GLN
1	A	589	GLN
1	A	682	GLN
1	A	706	HIS
1	A	712	GLN
1	A	737	ASN
1	A	744	GLN
1	A	759	ASN
1	A	780	GLN
1	A	856	ASN
1	B	132	GLN
1	B	136	ASN
1	B	141	ASN
1	B	179	GLN
1	B	227	GLN
1	B	240	ASN
1	B	320	GLN
1	B	377	ASN
1	B	401	GLN
1	B	408	GLN

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Mol	Chain	Res	Type
1	B	454	GLN
1	B	522	ASN
1	B	538	ASN
1	B	559	GLN
1	B	560	GLN
1	B	563	GLN
1	B	581	GLN
1	B	625	GLN
1	B	665	GLN
1	B	682	GLN
1	B	702	ASN
1	B	712	GLN
1	B	740	GLN
1	B	744	GLN
1	B	759	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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	871/876 (99%)	-0.21	25 (2%) 52 37	11, 51, 141, 200	1 (0%)
1	B	845/876 (96%)	0.58	89 (10%) 7 4	14, 102, 189, 199	0
2	C	36/40 (90%)	-0.15	0 100 100	31, 63, 103, 133	0
2	D	23/40 (57%)	0.66	4 (17%) 2 1	58, 70, 82, 90	0
All	All	1775/1832 (96%)	0.18	118 (6%) 19 11	11, 67, 178, 200	1 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	830	GLY	13.8
1	B	812	ASP	13.6
1	B	623	GLY	10.7
1	B	811	THR	10.6
1	B	800	PHE	10.2
1	B	803	HIS	9.5
1	B	790	VAL	8.6
1	A	876	ALA	8.4
1	B	813	GLY	8.3
1	B	809	ASP	7.7
2	D	62	ALA	7.5
1	B	622	GLY	7.2
1	A	781	GLU	6.9
1	B	487	VAL	6.4
1	B	620	GLY	6.2
1	B	163	PRO	5.9
1	B	791	GLN	5.9
1	B	807	ASP	5.8
1	B	621	SER	5.5
1	B	801	ILE	5.3
1	B	808	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	627	ASP	5.2
1	B	810	HIS	5.1
1	B	705	VAL	5.1
1	B	731	TYR	5.0
1	B	876	ALA	4.8
1	B	340	ASP	4.6
1	B	665	GLN	4.5
1	B	488	ALA	4.4
1	B	626	GLU	4.4
1	A	569	GLN	4.2
1	B	829	PHE	4.2
1	B	572	SER	4.2
1	B	822	ILE	4.2
1	A	623	GLY	4.1
1	B	831	LYS	4.1
1	B	490	ASP	4.1
1	A	306	PRO	4.1
1	B	706	HIS	4.0
1	B	160	ASP	3.9
2	D	59	VAL	3.8
1	A	779	ASP	3.7
1	B	850	GLY	3.7
1	B	167	GLN	3.7
1	A	780	GLN	3.7
1	B	788	MET	3.7
1	B	666	VAL	3.7
1	A	783	VAL	3.6
1	B	713	ILE	3.6
1	B	797	ILE	3.4
1	A	490	ASP	3.4
1	A	855	THR	3.4
1	B	486	ASP	3.4
1	A	624	VAL	3.4
1	B	612	LEU	3.4
2	D	63	ARG	3.4
1	B	653	PHE	3.3
1	B	702	ASN	3.2
1	A	487	VAL	3.2
1	B	742	ALA	3.2
1	A	488	ALA	3.2
1	A	336	ASN	3.2
1	A	874	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	491	GLN	3.1
1	A	854	LYS	3.0
1	B	657	GLY	3.0
1	A	301	ALA	3.0
1	B	796	PHE	3.0
1	B	817	CYS	3.0
1	A	335	GLU	3.0
1	B	624	VAL	2.9
1	B	804	ILE	2.9
1	B	602	GLN	2.9
1	B	717	PHE	2.8
1	B	846	LEU	2.7
1	B	652	PRO	2.7
1	B	141	ASN	2.7
1	B	738	THR	2.7
1	B	615	PHE	2.7
1	A	706	HIS	2.7
1	B	681	LEU	2.6
1	B	852	ARG	2.6
1	B	875	GLN	2.6
1	B	608	MET	2.6
1	B	625	GLN	2.6
1	B	309	HIS	2.6
1	A	782	ASN	2.6
1	A	305	ARG	2.5
1	B	306	PRO	2.5
1	B	845	GLU	2.5
1	B	826	CYS	2.5
1	B	561	VAL	2.5
1	B	815	VAL	2.5
1	B	842	MET	2.4
1	B	338	ASP	2.4
1	B	857	LYS	2.4
1	B	744	GLN	2.4
1	B	617	SER	2.3
1	B	761	LEU	2.3
1	B	729	LYS	2.3
1	B	560	GLN	2.3
1	B	619	ALA	2.3
1	A	486	ASP	2.2
1	B	164	GLU	2.2
2	D	58	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	340	ASP	2.2
1	A	492	GLU	2.2
1	B	95	VAL	2.1
1	B	81	LEU	2.1
1	B	1	MET	2.1
1	A	304	GLY	2.1
1	B	673	LEU	2.1
1	B	493	GLU	2.0
1	B	680	ALA	2.0
1	B	671	VAL	2.0
1	B	677	LEU	2.0
1	B	816	ALA	2.0
1	B	489	ASP	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.