



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:38 AM UTC

PDB ID : 2Q5D / pdb_00002q5d
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

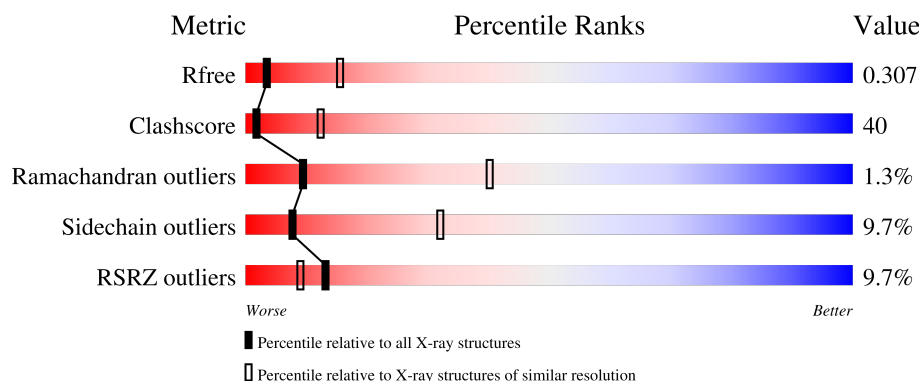
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	876	4% 57% 34% 7% ..
1	B	876	15% 47% 36% 12% ..
2	C	40	45% 38% 8% 10%
2	D	40	5% 48% 10% 42%

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			

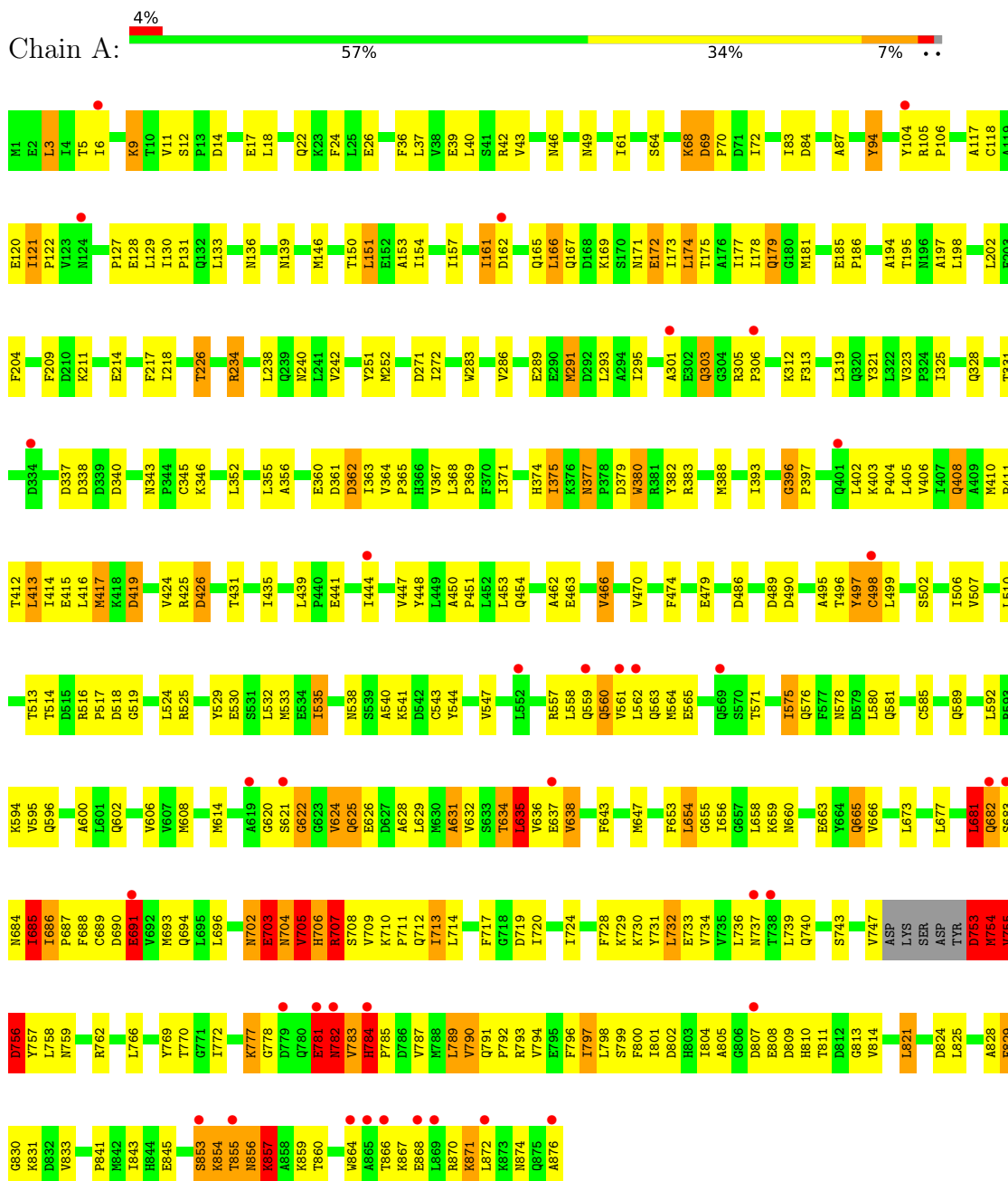
- Molecule 2 is a protein called Snurportin-1.

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			

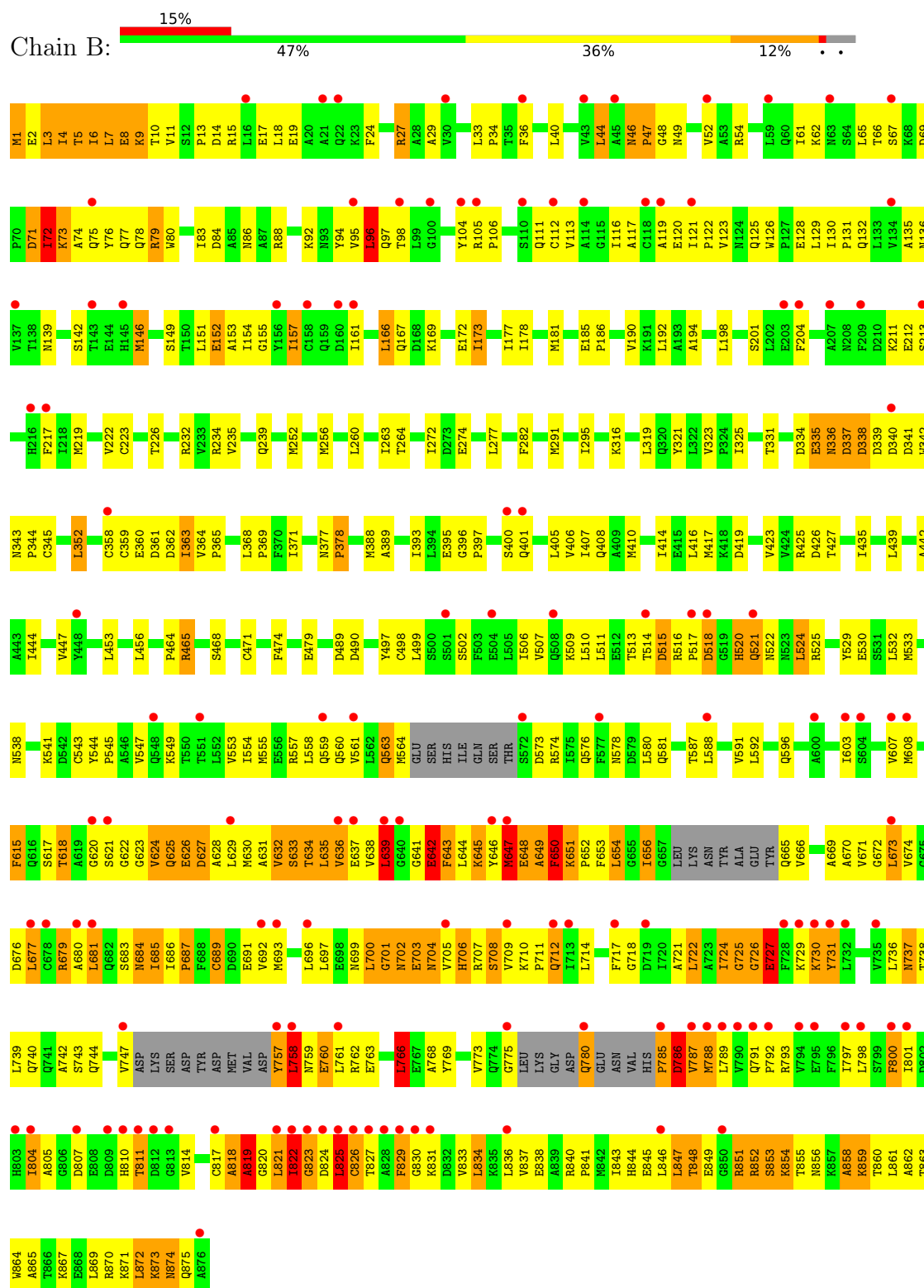
3 Residue-property plots

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

• Molecule 1: 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, α , β , γ	102.98Å 100.70Å 108.68Å 90.00° 109.23° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 91.2 (40.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.61	0/6871	1.04	39/9328 (0.4%)
1	B	0.55	0/6651	0.98	23/9023 (0.3%)
2	C	0.57	0/326	0.94	0/428
2	D	0.65	0/114	0.71	0/158
All	All	0.58	0/13962	1.00	62/18937 (0.3%)

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 (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	SER	CA-C-N	7.88	127.60	119.56
1	A	12	SER	C-N-CA	7.88	127.60	119.56
1	B	558	LEU	N-CA-C	-6.99	104.83	113.15
1	A	685	ILE	N-CA-C	-6.93	105.97	112.83
1	A	635	LEU	N-CA-C	-6.88	104.36	112.89
1	A	64	SER	N-CA-C	-6.83	104.49	114.39
1	B	8	GLU	N-CA-C	-6.82	103.84	111.28
1	A	691	GLU	N-CA-C	-6.77	103.83	111.14
1	B	447	VAL	N-CA-C	6.77	116.97	111.62
1	A	447	VAL	CB-CA-C	-6.68	105.11	111.05
1	A	466	VAL	CB-CA-C	-6.58	104.98	111.30
1	A	507	VAL	N-CA-C	6.53	117.21	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	844	HIS	N-CA-C	-6.42	105.31	113.01
1	B	869	LEU	N-CA-C	-6.34	105.20	113.12
1	A	575	ILE	N-CA-C	6.33	116.50	110.42
1	B	524	LEU	N-CA-C	6.32	117.83	111.07
1	A	866	THR	N-CA-C	-6.18	104.44	112.23
1	B	847	LEU	N-CA-C	-6.18	104.65	111.82
1	A	558	LEU	N-CA-C	-6.10	106.20	113.21
1	A	69	ASP	CA-C-N	6.08	125.79	119.05
1	A	69	ASP	C-N-CA	6.08	125.79	119.05
1	B	435	ILE	N-CA-C	-6.07	104.59	110.72
1	A	713	ILE	N-CA-C	-6.04	104.41	111.00
1	B	737	ASN	N-CA-C	-6.01	104.36	111.03
1	B	352	LEU	N-CA-C	-6.01	104.85	111.82
1	B	607	VAL	N-CA-C	5.97	116.09	110.30
1	A	94	TYR	N-CA-C	-5.97	104.74	112.68
1	A	151	LEU	N-CA-C	-5.92	105.55	112.89
1	B	819	ALA	N-CA-C	-5.88	105.25	113.37
1	A	303	GLN	N-CA-C	-5.81	105.97	114.39
1	B	152	GLU	N-CA-C	-5.76	104.98	112.23
1	A	283	TRP	N-CA-C	5.59	118.30	111.82
1	A	790	VAL	N-CA-C	-5.52	107.41	113.43
1	B	295	ILE	N-CA-C	-5.51	105.00	111.00
1	B	760	GLU	N-CA-C	-5.50	106.24	113.12
1	A	629	LEU	N-CA-C	-5.49	105.84	112.54
1	A	174	LEU	N-CA-C	5.47	118.00	111.71
1	A	271	ASP	N-CA-C	-5.46	106.62	113.72
1	A	337	ASP	N-CA-C	5.46	118.19	110.50
1	A	380	TRP	N-CA-C	5.41	117.87	111.33
1	B	507	VAL	N-CA-C	5.38	116.16	110.72
1	A	784	HIS	CA-C-N	5.38	127.55	121.04
1	A	784	HIS	C-N-CA	5.38	127.55	121.04
1	B	656	ILE	CB-CA-C	-5.27	102.65	111.29
1	B	818	ALA	N-CA-C	-5.26	105.19	111.03
1	B	766	LEU	N-CA-C	-5.25	105.63	111.36
1	A	291	MET	N-CA-C	-5.25	104.48	112.04
1	B	615	PHE	N-CA-C	5.24	116.67	111.07
1	A	789	LEU	N-CA-C	-5.18	106.91	113.18
1	A	139	ASN	CA-C-N	5.18	124.84	119.56
1	A	139	ASN	C-N-CA	5.18	124.84	119.56
1	B	345	CYS	N-CA-C	5.16	116.91	111.28
1	B	61	ILE	CB-CA-C	-5.16	105.17	112.14
1	A	286	VAL	N-CA-C	-5.13	105.50	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	717	PHE	N-CA-C	-5.11	105.83	111.71
1	A	543	CYS	N-CA-C	-5.08	106.00	113.61
1	A	295	ILE	N-CA-C	-5.07	106.20	111.58
1	A	631	ALA	N-CA-C	-5.06	105.46	111.69
1	A	87	ALA	N-CA-C	-5.06	105.77	111.28
1	A	226	THR	N-CA-C	-5.04	106.91	113.16
1	A	419	ASP	N-CA-C	5.03	116.02	109.64
1	B	291	MET	N-CA-C	-5.02	105.47	112.45

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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	449	0
1	B	6550	0	6568	688	0
2	C	323	0	337	16	0
2	D	115	0	48	7	0
All	All	13750	0	13717	1103	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 40.

All (1103) 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
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:562:LEU:O	1:A:562:LEU:HD23	1.46	1.15
1:A:781:GLU:O	1:B:573:ASP:HB2	1.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:130:ILE:CG2	1:A:131:PRO:CD	2.27	1.12
1:A:561:VAL:HA	1:A:564:MET:HG3	1.25	1.12
1:A:704:ASN:HB2	1:A:705:VAL:HG22	1.23	1.12
1:B:647:MET:C	1:B:649:ALA:HB2	1.73	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:69:ASP:HB2	1:B:72:ILE:CG2	1.82	1.09
1:B:130:ILE:HG13	1:B:131:PRO:CD	1.81	1.09
1:A:737:ASN:HD22	1:B:13:PRO:HA	0.92	1.08
1:B:96:LEU:HD21	1:B:132:GLN:HG2	1.23	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:634:THR:O	1:B:638:VAL:HG23	1.51	1.07
1:A:783:VAL:C	1:A:785:PRO:HD3	1.78	1.07
1:B:819:ALA:C	1:B:822:ILE:HG23	1.78	1.06
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:819:ALA:C	1:B:822:ILE:CG2	2.31	1.04
1:A:783:VAL:O	1:A:785:PRO:HD3	1.58	1.03
1:B:681:LEU:HD13	1:B:685:ILE:HG22	1.04	1.03
1:B:69:ASP:HB2	1:B:72:ILE:HG23	1.38	1.03
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
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:1:MET:HE3	1:B:2:GLU:O	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:B:685:ILE:H	1.28	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:B:679:ARG:HG3	1:B:679:ARG:HH11	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
1:A:375:ILE:HD13	1:A:375:ILE:O	1.67	0.93
1:A:561:VAL:HG22	1:A:564:MET:HE3	1.48	0.93
1:B:644:LEU:HD12	1:B:644:LEU:O	1.68	0.93
1:B:649:ALA:HA	1:B:650:PHE:CD2	2.03	0.93
1:A:777:LYS:HG2	1:A:778:GLY:N	1.79	0.93
1:B:727:GLU:CD	1:B:727:GLU:H	1.75	0.93
1:B:848:THR:HG23	1:B:851:ARG:HH21	1.31	0.92
1:B:560:GLN:HG2	1:B:564:MET:HE3	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	1:B:712:GLN:HA	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:388:MET:HE1	2:C:32:LYS:HE3	1.54	0.88
1:A:3:LEU:HA	1:A:6:ILE:CD1	2.04	0.88
1:B:11:VAL:HG21	1:B:52:VAL:HG11	1.54	0.88
1:B:825:LEU:N	1:B:825:LEU:HD23	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:5:THR:HG22	1:B:5:THR:O	1.72	0.86
1:B:516:ARG:NH2	1:B:524:LEU:HD13	1.89	0.86
1:B:671:VAL:HG11	1:B:709:VAL:HG13	1.55	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASN:HD22	1:B:378:PRO:CD	1.89	0.85
1:A:856:ASN:C	1:A:857:LYS:HG2	2.00	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:HH11	1:B:27:ARG:HG3	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:759:ASN:ND2	1:B:814:VAL:HG13	1.93	0.83
1:B:766:LEU:HD13	1:B:821:LEU:HB2	1.59	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:778:GLY:HA3	1:A:781:GLU:CD	2.04	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: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: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
1:B:826:CYS:SG	1:B:865:ALA:CA	2.68	0.81
1:A:706:HIS:O	1:A:706:HIS:CD2	2.34	0.80
1:B:644:LEU:CD1	1:B:684:ASN:HD21	1.94	0.80
1:B:1:MET:HB3	1:B:2:GLU:C	2.06	0.80
1:B:649:ALA:C	1:B:650:PHE:CD2	2.60	0.80
1:B:787:VAL:HB	1:B:789:LEU:HD11	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:852:ARG:HG3	1:B:852:ARG:NH1	1.96	0.80
1:B:5:THR:O	1:B:5:THR:CG2	2.30	0.80
1:B:647:MET:C	1:B:649:ALA:CB	2.53	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:A:561:VAL:HG22	1:A:564:MET:CE	2.12	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: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:626:GLU:C	1:B:628:ALA:H	1.91	0.78
1:A:870:ARG:NH2	1:B:277:LEU:HD22	1.98	0.77
1:B:181:MET:HE1	1:B:198:LEU:HD22	1.66	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: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
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:B:641:GLY:C	1:B:642:GLU:HG3	2.09	0.75
1:A:870:ARG:HG3	1:B:342:TRP:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:819:ALA:C	1:B:822:ILE:HG21	2.13	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:530:GLU:HA	1:A:533:MET:HE2	1.71	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: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:B:818:ALA:C	1:B:820:GLY:H	1.97	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:A:653:PHE:HA	1:A:656:ILE:HG22	1.73	0.71
1:B:96:LEU:HD21	1:B:132:GLN:CG	2.13	0.71
1:B:762:ARG:HD2	1:B:800:PHE:CE1	2.24	0.71
1:B:727:GLU:CD	1:B:727:GLU:N	2.44	0.71
1:A:825:LEU:O	1:A:829:PHE:HB2	1.91	0.71
1:B:3:LEU:C	1:B:6:ILE:HG22	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:337:ASP:O	1:B:338:ASP:C	2.33	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:841:PRO:HB2	1:B:232:ARG:NH1	2.07	0.69
1:A:870:ARG:CG	1:B:342:TRP:HB3	2.22	0.69
1:A:782:ASN:CA	1:B:574:ARG:HB2	2.21	0.69
1:B:235:VAL:HG21	1:B:274:GLU:HG3	1.75	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: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: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: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:B:136:ASN:HB3	1:B:146:MET:HE2	1.76	0.67
1:A:179:GLN:HE21	1:A:179:GLN:HA	1.60	0.67
1:A:181:MET:HE1	1:A:198:LEU:HD22	1.75	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:PRO:HB2	1:A:402:LEU:HD11	1.76	0.67
1:B:679:ARG:HG3	1:B:679:ARG:NH1	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:A:561:VAL:CG2	1:A:564:MET:HE3	2.22	0.66
1:B:71:ASP:O	1:B:74:ALA:N	2.29	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:A:782:ASN:N	1:A:782:ASN:HD22	1.94	0.66
1:A:755:VAL:C	1:A:757:TYR:H	2.02	0.66
1:B:626:GLU:C	1:B:628:ALA:N	2.50	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:A:177:ILE:HG22	1:A:181:MET:HE2	1.78	0.65
1:A:565:GLU:CD	1:A:624:VAL:CG1	2.70	0.65
1:B:92:LYS:HD3	1:B:120:GLU:OE2	1.95	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:A:608:MET:HE3	1:A:643:PHE:HE1	1.62	0.65
1:B:516:ARG:NE	1:B:518:ASP:HB3	2.12	0.65
1:A:867:LYS:HG3	1:B:341:ASP:CG	2.21	0.65
1:B:46:ASN:O	1:B:49:ASN:HB2	1.96	0.65
1:A:783:VAL:H	1:B:574:ARG:HB2	1.61	0.65
1:A:811:THR:HG23	1:A:814:VAL:HG23	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:N	1:A:782:ASN:ND2	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:636:VAL:HG12	1:A:636:VAL:O	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: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:867:LYS:NZ	1:B:334:ASP:OD2	2.33	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: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:B:167:GLN:HG2	1:B:204:PHE:HB2	1.82	0.60
1:B:96:LEU:CD2	1:B:132:GLN:HG2	2.15	0.60
1:B:123:VAL:HG23	1:B:125:GLN:HB2	1.83	0.60
1:B:825:LEU:N	1:B:825:LEU:CD2	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:818:ALA:C	1:B:820:GLY:N	2.58	0.60
1:B:848:THR:HG23	1:B:851:ARG:NH2	2.10	0.60
1:B:377:ASN:HD22	1:B:377:ASN:C	2.09	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:67:SER:CB	1:B:72:ILE:O	2.50	0.59
1:B:645:LYS:O	1:B:645:LYS:HG2	2.00	0.59
1:A:712:GLN:HA	1:A:712:GLN:HE21	1.67	0.59
1:A:755:VAL:O	1:A:757:TYR:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:706:HIS:HD2	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:83:ILE:HG22	1:A:84:ASP:N	2.18	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:B:395:GLU:C	1:B:397:PRO:CD	2.76	0.58
1:A:871:LYS:CG	1:B:340:ASP:HA	2.32	0.58
1:B:94:TYR:O	1:B:97:GLN:N	2.33	0.58
1:B:683:SER:O	1:B:685:ILE:CD1	2.50	0.58
1:B:151:LEU:HD13	1:B:194:ALA:HB2	1.85	0.58
1:B:161:ILE:HG21	1:B:166:LEU:HD12	1.83	0.58
1:B:617:SER:O	1:B:618:THR:HG23	2.03	0.58
1:A:831:LYS:HE2	1:A:876:ALA:CB	2.31	0.58
1:A:857:LYS:HA	1:A:860:THR:HG23	1.84	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:681:LEU:HD12	1:B:681:LEU:H	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:HG12	1:B:833:VAL:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ARG:C	1:B:559:GLN:H	2.10	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:561:VAL:HG13	1:A:564:MET:HE3	1.87	0.57
1:A:589:GLN:CG	1:A:634:THR:HG21	2.33	0.57
1:A:608:MET:HE1	1:A:632:VAL:HG13	1.86	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:A:3:LEU:HD13	1:A:6:ILE:HD11	1.86	0.57
1:A:130:ILE:HD11	1:A:172:GLU:CB	2.35	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:B:786:ASP:CG	1:B:787:VAL:N	2.63	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: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:581:GLN:HE22	1:B:628:ALA:HB1	1.70	0.56
1:B:758:LEU:O	1:B:760:GLU:N	2.39	0.56
1:A:120:GLU:C	1:A:122:PRO:HD2	2.29	0.56
1:B:319:LEU:O	1:B:323:VAL:HG23	2.06	0.56
1:B:683:SER:C	1:B:685:ILE:HD12	2.30	0.56
1:B:829:PHE:HB2	1:B:833:VAL:CG2	2.35	0.56
1:B:46:ASN:O	1:B:49:ASN:HB3	2.05	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: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:B:46:ASN:C	1:B:49:ASN:HB2	2.31	0.56
1:A:743:SER:HB3	1:A:800:PHE:CD1	2.41	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:331:THR:O	1:B:331:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:14:ASP:HB3	1:B:17:GLU:HB3	1.88	0.55
1:B:62:LYS:O	1:B:66:THR:HG22	2.06	0.55
1:B:416:LEU:O	1:B:419:ASP:HB2	2.05	0.55
1:A:782:ASN:CB	1:B:574:ARG:CA	2.80	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:720:ILE:CG2	1:A:724:ILE:HD13	2.30	0.55
1:A:856:ASN:C	1:A:857:LYS:CG	2.78	0.55
1:B:646:TYR:O	1:B:648:GLU:N	2.40	0.55
1:B:651:LYS:HE2	1:B:691:GLU:CD	2.32	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:O	1:A:707:ARG:HG3	2.05	0.55
1:A:565:GLU:OE1	1:A:624:VAL:HG11	2.07	0.55
1:B:7:LEU:HA	1:B:10:THR:HG23	1.87	0.55
1:B:46:ASN:O	1:B:54:ARG:HD2	2.07	0.55
1:B:121:ILE:N	1:B:122:PRO:HD2	2.21	0.55
1:B:563:GLN:C	1:B:563:GLN:HE21	2.14	0.55
1:B:683:SER:C	1:B:685:ILE:CD1	2.80	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:A:693:MET:HE3	1:A:720:ILE:HG21	1.89	0.55
1:B:27:ARG:HG3	1:B:27:ARG:NH1	2.18	0.55
1:B:530:GLU:HA	1:B:533:MET:HE2	1.89	0.55
1:B:821:LEU:C	1:B:824:ASP:HB2	2.32	0.55
1:B:679:ARG:NH1	1:B:679:ARG:CG	2.66	0.55
1:B:763:GLU:HB2	1:B:817:CYS:HB3	1.87	0.55
1:B:800:PHE:CD1	1:B:800:PHE:C	2.85	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:A:798:LEU:C	1:A:801:ILE:HG12	2.32	0.54
1:B:129:LEU:O	1:B:132:GLN:HB3	2.08	0.54
1:A:753:ASP:CG	1:A:753:ASP:O	2.49	0.54
1:B:639:LEU:HD13	1:B:643:PHE:HZ	1.72	0.54
1:A:362:ASP:OD1	1:A:362:ASP:N	2.34	0.54
1:B:578:ASN:OD1	1:B:624:VAL:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:LEU:HD23	1:A:801:ILE:CD1	2.38	0.54
1:A:857:LYS:HA	1:A:860:THR:OG1	2.08	0.54
1:B:649:ALA:C	1:B:650:PHE:CG	2.85	0.54
1:B:831:LYS:O	1:B:834:LEU:HB3	2.07	0.54
1:B:851:ARG:O	1:B:852:ARG:HB2	2.06	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:766:LEU:HA	1:B:769:TYR:HD2	1.73	0.54
1:B:651:LYS:HD3	1:B:691:GLU:CD	2.33	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:360:GLU:O	1:A:361:ASP:C	2.51	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:818:ALA:C	1:B:846:LEU:HD11	2.34	0.53
1:B:46:ASN:OD1	1:B:47:PRO:HD2	2.09	0.53
1:B:364:VAL:N	1:B:365:PRO:CD	2.71	0.53
1:B:759:ASN:ND2	1:B:817:CYS:HB2	2.24	0.53
1:B:831:LYS:N	1:B:872:LEU:HD12	2.24	0.53
1:B:852:ARG:O	1:B:854:LYS:HE2	2.09	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:69:ASP:CB	1:A:72:ILE:HD12	2.39	0.53
1:A:705:VAL:HG12	1:A:706:HIS:CB	2.34	0.53
1:B:5:THR:O	1:B:9:LYS:HG2	2.09	0.53
1:B:775:GLY:C	1:B:780:GLN:N	2.67	0.53
1:A:755:VAL:C	1:A:757:TYR:N	2.63	0.53
1:B:766:LEU:CD1	1:B:821:LEU:HB2	2.34	0.53
1:B:377:ASN:ND2	1:B:377:ASN:C	2.66	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
2:C:61:HIS:ND1	2:C:61:HIS:C	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:ARG:O	1:B:757:TYR:OH	2.27	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:6:ILE:HG23	1:B:7:LEU:N	2.22	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:N	1:A:128:GLU:OE1	2.42	0.52
1:A:707:ARG:O	1:A:707:ARG:CG	2.54	0.52
1:A:559:GLN:C	1:A:561:VAL:N	2.66	0.52
2:C:50:LEU:O	2:C:54:LYS:HG2	2.10	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
1:A:174:LEU:O	1:A:178:ILE:HG12	2.09	0.52
1:A:703:GLU:O	1:A:703:GLU:HG3	2.08	0.52
1:B:44:LEU:HG	1:B:98:THR:OG1	2.10	0.52
1:B:71:ASP:O	1:B:73:LYS:N	2.43	0.52
1:B:464:PRO:CA	1:B:524:LEU:HD12	2.40	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:807:ASP:C	1:A:809:ASP:H	2.17	0.52
1:B:824:ASP:C	1:B:826:CYS:H	2.18	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:444:ILE:HD12	1:A:444:ILE:H	1.75	0.51
1:A:559:GLN:O	1:A:561:VAL:N	2.43	0.51
1:B:75:GLN:O	1:B:79:ARG:HB2	2.10	0.51
1:B:736:LEU:HD13	1:B:793:ARG:CZ	2.40	0.51
1:B:834:LEU:HD21	1:B:873:LYS:HB3	1.92	0.51
1:B:843:ILE:C	1:B:845:GLU:N	2.68	0.51
1:B:843:ILE:C	1:B:845:GLU:H	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASP:C	1:A:340:ASP:H	2.18	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
2:C:60:ASN:HA	2:C:63:ARG:HG3	1.93	0.51
1:B:651:LYS:O	1:B:654:LEU:HB2	2.11	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:84:ASP:OD2	1:B:86:ASN:HB2	2.11	0.51
1:B:173:ILE:CD1	1:B:173:ILE:H	2.24	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:559:GLN:C	1:A:561:VAL:H	2.18	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:3:LEU:O	1:A:6:ILE:HG12	2.11	0.50
1:A:6:ILE:CD1	1:A:24:PHE:HE1	2.24	0.50
1:B:223:CYS:O	1:B:226:THR:OG1	2.30	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:B:791:GLN:N	1:B:792:PRO:HD2	2.26	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:A:787:VAL:C	1:A:789:LEU:H	2.20	0.50
1:B:72:ILE:HG23	1:B:72:ILE:O	2.11	0.50
1:B:6:ILE:O	1:B:9:LYS:HB2	2.12	0.50
1:B:395:GLU:C	1:B:397:PRO:HD2	2.37	0.50
1:B:681:LEU:HD12	1:B:681:LEU:N	2.26	0.50
1:A:867:LYS:HE3	1:B:341:ASP:HB2	1.93	0.50
1:B:518:ASP:OD2	1:B:518:ASP:C	2.55	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:560:GLN:O	1:B:564:MET:HE3	2.11	0.50
1:B:819:ALA:O	1:B:822:ILE:CG2	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLN:O	1:A:331:THR:HB	2.12	0.49
1:A:331:THR:HG22	1:A:331:THR:O	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:581:GLN:NE2	1:B:628:ALA:CB	2.75	0.49
1:B:588:LEU:HA	1:B:591:VAL:HG22	1.93	0.49
1:B:738:THR:HG22	1:B:761:LEU:HD21	1.94	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:5:THR:O	1:A:9:LYS:HG2	2.11	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
1:B:222:VAL:O	1:B:226:THR:HG23	2.12	0.49
1:B:272:ILE:N	1:B:272:ILE:HD12	2.28	0.49
1:A:39:GLU:O	1:A:43:VAL:HG23	2.12	0.49
1:A:319:LEU:HD12	1:A:355:LEU:HD22	1.92	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:486:ASP:CG	1:A:486:ASP:O	2.56	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:B:826:CYS:SG	1:B:865:ALA:C	2.95	0.49
1:A:136:ASN:HB3	1:A:146:MET:HE2	1.95	0.49
1:A:753:ASP:O	1:A:753:ASP:OD2	2.30	0.49
1:A:841:PRO:HB3	1:B:192:LEU:CD2	2.43	0.49
1:A:870:ARG:HH21	1:B:277:LEU:HD13	1.78	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:649:ALA:O	1:B:650:PHE:C	2.56	0.49
1:A:377:ASN:ND2	1:A:379:ASP:H	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:O	1:B:73:LYS:HG3	2.12	0.49
1:B:465:ARG:HG2	1:B:522:ASN:ND2	2.27	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:425:ARG:NH2	1:A:463:GLU:OE1	2.46	0.48
1:B:95:VAL:C	1:B:97:GLN:H	2.21	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:834:LEU:CD2	1:B:873:LYS:HB3	2.43	0.48
1:B:845:GLU:O	1:B:849:GLU:N	2.37	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
1:A:625:GLN:O	1:A:666:VAL:HG13	2.13	0.48
1:B:69:ASP:CB	1:B:72:ILE:CG2	2.74	0.48
1:B:72:ILE:O	1:B:72:ILE:HG12	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:787:VAL:C	1:B:789:LEU:HG	2.38	0.48
1:A:513:THR:HG23	1:A:516:ARG:HD3	1.95	0.48
1:A:706:HIS:CD2	1:A:706:HIS:C	2.89	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:A:375:ILE:HD13	1:A:375:ILE:C	2.37	0.48
1:A:419:ASP:O	1:A:425:ARG:HD3	2.13	0.48
1:A:706:HIS:O	1:A:706:HIS:CG	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:707:ARG:C	1:B:709:VAL:N	2.70	0.48
1:B:773:VAL:C	1:B:775:GLY:H	2.22	0.48
1:B:829:PHE:HB2	1:B:833:VAL:HG23	1.96	0.48
1:A:513:THR:HA	1:A:516:ARG:HG3	1.95	0.48
1:B:707:ARG:N	1:B:707:ARG:CD	2.77	0.48
1:A:682:GLN:HE21	1:A:682:GLN:HB2	1.53	0.47
1:A:209:PHE:C	1:A:211:LYS:H	2.23	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:557:ARG:C	1:A:559:GLN:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:THR:HB	1:B:529:TYR:CZ	2.49	0.47
1:B:615:PHE:HA	1:B:625:GLN:HE21	1.79	0.47
1:B:759:ASN:ND2	1:B:814:VAL:C	2.72	0.47
1:B:768:ALA:O	1:B:769:TYR:C	2.57	0.47
1:A:663:GLU:C	1:A:665:GLN:H	2.22	0.47
1:A:782:ASN:HD22	1:A:782:ASN:H	1.62	0.47
1:B:132:GLN:HE21	1:B:136:ASN:HD21	1.62	0.47
1:B:786:ASP:CG	1:B:787:VAL:H	2.22	0.47
1:A:375:ILE:HD11	1:A:412:THR:HG22	1.97	0.47
1:B:851:ARG:O	1:B:852:ARG:CB	2.62	0.47
1:A:312:LYS:O	1:A:313:PHE:C	2.57	0.47
1:A:728:PHE:O	1:A:729:LYS:C	2.57	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: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:1:MET:HB2	1:B:3:LEU:HD21	1.93	0.47
1:B:19:GLU:OE2	1:B:19:GLU:HA	2.13	0.47
1:B:130:ILE:CG1	1:B:131:PRO:HD2	2.09	0.47
1:B:149:SER:O	1:B:152:GLU:HB2	2.15	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:B:712:GLN:HA	1:B:712:GLN:NE2	2.15	0.47
1:B:71:ASP:C	1:B:73:LYS:H	2.23	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:859:LYS:O	1:B:863:THR:HB	2.15	0.47
1:A:712:GLN:HA	1:A:712:GLN:NE2	2.29	0.47
1:B:117:ALA:C	1:B:119:ALA:H	2.23	0.47
1:B:453:LEU:HD21	1:B:499:LEU:CD2	2.43	0.47
1:B:641:GLY:C	1:B:642:GLU:CG	2.85	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:561:VAL:CB	1:A:564:MET:HE3	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:301:ALA:C	1:A:303:GLN:H	2.22	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
2:C:27:ARG:O	2:C:29:SER:N	2.48	0.46
1:B:620:GLY:O	1:B:621:SER:HB2	2.14	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:426:ASP:OD1	1:A:426:ASP:C	2.58	0.46
1:A:565:GLU:CD	1:A:624:VAL:HG13	2.39	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:565:GLU:CD	1:A:624:VAL:HG11	2.39	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:HD13	1:B:804:ILE:HA	1.88	0.46
1:A:731:TYR:C	1:A:733:GLU:N	2.72	0.46
1:B:554:ILE:HD13	1:B:587:THR:HG22	1.96	0.46
1:B:702:ASN:O	1:B:703:GLU:C	2.59	0.46
1:B:853:SER:C	1:B:854:LYS:HD3	2.40	0.46
1:A:777:LYS:HB2	1:A:787:VAL:CG1	2.43	0.46
1:B:362:ASP:OD1	1:B:362:ASP:N	2.49	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:ND2	1:A:856:ASN:H	2.14	0.46
1:B:841:PRO:C	1:B:843:ILE:H	2.23	0.46
1:A:871:LYS:HZ2	1:A:874:ASN:HB2	1.80	0.46
1:B:27:ARG:CG	1:B:27:ARG:NH1	2.76	0.46
1:B:557:ARG:C	1:B:559:GLN:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:LEU:O	2:D:60:ASN:N	2.49	0.45
1:A:83:ILE:CG2	1:A:84:ASP:N	2.79	0.45
1:A:305:ARG:HA	1:A:306:PRO:HD3	1.85	0.45
1:B:83:ILE:O	1:B:84:ASP:C	2.58	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:513:THR:HA	1:B:516:ARG:HD3	1.97	0.45
1:B:560:GLN:C	1:B:564:MET:HE3	2.42	0.45
1:A:117:ALA:O	1:A:121:ILE:HD13	2.16	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:A:709:VAL:O	1:A:710:LYS:C	2.59	0.45
1:A:867:LYS:CE	1:B:341:ASP:CG	2.89	0.45
1:B:335:GLU:C	1:B:335:GLU:CD	2.85	0.45
1:B:444:ILE:HD12	1:B:498:CYS:SG	2.56	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:3:LEU:C	1:A:6:ILE:HG12	2.41	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
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:A:787:VAL:C	1:A:789:LEU:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:272:ILE:HD12	2.32	0.45
1:A:331:THR:HG21	1:A:382:TYR:CZ	2.52	0.45
1:A:790:VAL:C	1:A:792:PRO:HD2	2.42	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:592:LEU:C	1:A:594:LYS:H	2.23	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:B:834:LEU:CD1	1:B:834:LEU:C	2.90	0.44
1:A:374:HIS:HB3	1:A:382:TYR:O	2.17	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:672:GLY:O	1:B:673:LEU:C	2.60	0.44
1:B:699:ASN:C	1:B:701:GLY:N	2.75	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:A:731:TYR:O	1:A:733:GLU:N	2.51	0.44
1:A:737:ASN:ND2	1:B:13:PRO:C	2.76	0.44
1:A:753:ASP:HA	1:A:755:VAL:HG13	1.99	0.44
1:B:608:MET:HE1	1:B:632:VAL:HG13	1.98	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:252:MET:HE2	1:A:252:MET:HA	2.00	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:A:517:PRO:C	1:A:519:GLY:H	2.25	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
1:B:824:ASP:C	1:B:826:CYS:N	2.75	0.44
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
2:C:49:GLU:HG3	2:C:50:LEU:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:650:PHE:HA	1:B:652:PRO:HD2	2.00	0.44
2:C:55:ARG:O	2:C:59:VAL:HG23	2.18	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:801:ILE:HG21	1:B:846:LEU:HD13	2.00	0.44
1:B:805:ALA:C	1:B:810:HIS:NE2	2.76	0.44
1:A:133:LEU:HD22	1:A:150:THR:HG23	2.00	0.43
1:B:2:GLU:CD	1:B:4:ILE:HD11	2.43	0.43
1:A:167:GLN:HG2	1:A:204:PHE:HB2	1.98	0.43
1:A:415:GLU:C	1:A:417:MET:N	2.74	0.43
1:A:635:LEU:HD12	1:A:635:LEU:HA	1.81	0.43
1:A:653:PHE:C	1:A:655:GLY:H	2.26	0.43
1:B:670:ALA:O	1:B:673:LEU:N	2.51	0.43
1:A:415:GLU:C	1:A:417:MET:H	2.27	0.43
1:A:628:ALA:O	1:A:632:VAL:HG23	2.17	0.43
1:A:712:GLN:HE21	1:A:712:GLN:CA	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:676:ASP:O	1:B:677:LEU:C	2.60	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:A:706:HIS:CA	1:A:707:ARG:HB3	2.40	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:O	1:A:375:ILE:CD1	2.54	0.43
1:B:560:GLN:HE21	1:B:564:MET:HE1	1.83	0.43
1:B:834:LEU:HD21	1:B:873:LYS:CG	2.47	0.43
1:A:403:LYS:N	1:A:404:PRO:HD2	2.33	0.43
1:B:94:TYR:O	1:B:97:GLN:CB	2.65	0.43
1:A:663:GLU:C	1:A:665:GLN:N	2.75	0.43
1:A:783:VAL:N	1:B:574:ARG:CB	2.75	0.43
1:B:371:ILE:CD1	1:B:389:ALA:HB3	2.48	0.43
1:A:69:ASP:HB3	1:A:72:ILE:HD12	2.00	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:802:ASP:HA	1:A:843:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LEU:CB	1:B:6:ILE:CG2	2.80	0.43
1:B:153:ALA:C	1:B:155:GLY:N	2.75	0.43
1:B:444:ILE:HG22	1:B:444:ILE:O	2.18	0.43
1:A:69:ASP:CG	1:A:72:ILE:HD12	2.44	0.43
1:A:653:PHE:C	1:A:655:GLY:N	2.76	0.43
1:B:73:LYS:O	1:B:77:GLN:HG3	2.19	0.43
1:B:773:VAL:C	1:B:775:GLY:N	2.75	0.43
1:A:42:ARG:NH1	1:A:94:TYR:OH	2.51	0.43
1:A:411:PRO:O	1:A:415:GLU:HG3	2.18	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:A:867:LYS:NZ	1:B:341:ASP:CG	2.77	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:A:291:MET:C	1:A:293:LEU:N	2.77	0.42
1:A:559:GLN:O	1:A:560:GLN:C	2.61	0.42
1:A:770:THR:HG23	1:A:824:ASP:OD2	2.19	0.42
1:B:112:CYS:O	1:B:113:VAL:C	2.62	0.42
1:B:135:ALA:O	1:B:139:ASN:HB2	2.19	0.42
1:B:343:ASN:O	1:B:344:PRO:C	2.61	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
2:D:57:ASP:C	2:D:60:ASN:H	2.27	0.42
1:A:154:ILE:H	1:A:154:ILE:HG13	1.59	0.42
1:A:729:LYS:O	1:A:730:LYS:C	2.61	0.42
1:A:841:PRO:HB2	1:B:232:ARG:HH11	1.81	0.42
1:B:76:TYR:N	1:B:76:TYR:CD1	2.85	0.42
1:B:361:ASP:OD1	1:B:401:GLN:NE2	2.53	0.42
1:B:683:SER:C	1:B:685:ILE:H	2.26	0.42
1:B:697:LEU:HD11	1:B:730:LYS:HE3	2.01	0.42
1:B:788:MET:HE1	1:B:791:GLN:HG3	2.01	0.42
1:A:127:PRO:HG2	1:A:128:GLU:OE1	2.19	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
2:C:27:ARG:C	2:C:29:SER:N	2.76	0.42
1:A:121:ILE:N	1:A:121:ILE:CD1	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:3:LEU:CA	1:B:6:ILE:HG22	2.49	0.42
1:B:388:MET:HB2	1:B:427:THR:HG21	2.02	0.42
1:B:708:SER:O	1:B:711:PRO:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:39:GLU:HG2	2:C:40:GLN:H	1.83	0.42
1:B:683:SER:O	1:B:685:ILE:N	2.50	0.42
1:B:820:GLY:C	1:B:822:ILE:H	2.28	0.42
1:B:834:LEU:CG	1:B:873:LYS:HB3	2.50	0.42
1:B:219:MET:HE2	1:B:252:MET:HE1	2.01	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:A:214:GLU:O	1:A:218:ILE:HG12	2.20	0.42
1:B:95:VAL:C	1:B:97:GLN:N	2.75	0.42
1:B:211:LYS:O	1:B:212:GLU:C	2.61	0.42
1:B:407:ILE:HD11	1:B:442:ALA:HA	2.00	0.42
1:A:291:MET:C	1:A:293:LEU:H	2.28	0.42
1:B:331:THR:O	1:B:331:THR:CG2	2.67	0.42
1:B:361:ASP:O	1:B:362:ASP:C	2.63	0.42
1:B:393:ILE:HD12	1:B:393:ILE:C	2.45	0.42
1:B:636:VAL:O	1:B:636:VAL:HG13	2.19	0.42
1:B:856:ASN:C	1:B:858:ALA:H	2.28	0.42
1:A:3:LEU:HA	1:A:6:ILE:CG1	2.49	0.42
1:A:173:ILE:HD12	1:A:173:ILE:N	2.35	0.42
1:B:173:ILE:N	1:B:173:ILE:HD12	2.35	0.42
1:B:198:LEU:HA	1:B:201:SER:HG	1.85	0.42
1:B:235:VAL:HG21	1:B:274:GLU:CG	2.47	0.42
1:B:426:ASP:OD1	1:B:426:ASP:C	2.62	0.42
1:A:153:ALA:O	1:A:157:ILE:HG13	2.20	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:68:LYS:HE3	1:A:68:LYS:N	2.35	0.41
1:A:375:ILE:HD11	1:A:416:LEU:HD11	2.01	0.41
1:A:782:ASN:C	1:B:574:ARG:HB2	2.46	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:B:834:LEU:C	1:B:834:LEU:HD13	2.45	0.41
1:A:544:TYR:O	1:A:547:VAL:N	2.51	0.41
1:A:660:ASN:OD1	1:A:660:ASN:C	2.61	0.41
1:B:71:ASP:C	1:B:73:LYS:N	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:852:ARG:HH11	1:B:852:ARG:CG	2.12	0.41
1:A:557:ARG:O	1:A:561:VAL:HG23	2.20	0.41
1:A:561:VAL:CG1	1:A:564:MET:HE3	2.49	0.41
2:C:42:GLU:O	2:C:43:ARG:C	2.61	0.41
1:B:69:ASP:CB	1:B:72:ILE:HG22	2.46	0.41
1:B:465:ARG:HG2	1:B:522:ASN:HD21	1.85	0.41
1:B:763:GLU:HA	1:B:766:LEU:CD1	2.51	0.41
1:A:793:ARG:O	1:A:794:VAL:C	2.62	0.41
1:B:65:LEU:HD13	1:B:116:ILE:CG1	2.48	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: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:HD23	1:A:677:LEU:HA	1.94	0.41
1:A:731:TYR:O	1:A:732:LEU:C	2.63	0.41
1:B:730:LYS:HB3	1:B:731:TYR:CD1	2.55	0.41
1:B:854:LYS:O	1:B:855:THR:OG1	2.30	0.41
1:A:3:LEU:CD2	1:A:6:ILE:HD11	2.48	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:364:VAL:HB	1:B:365:PRO:HD3	2.03	0.41
1:B:541:LYS:C	1:B:543:CYS:H	2.29	0.41
1:B:626:GLU:OE1	1:B:666:VAL:HG22	2.21	0.41
1:B:644:LEU:O	1:B:644:LEU:CG	2.69	0.41
1:B:680:ALA:HB1	1:B:681:LEU:HD12	2.01	0.41
1:B:693:MET:HE3	1:B:731:TYR:OH	2.21	0.41
1:B:738:THR:O	1:B:742:ALA:CB	2.68	0.41
1:B:824:ASP:O	1:B:825:LEU:C	2.64	0.41
1:A:497:TYR:HD1	1:A:497:TYR:H	1.69	0.41
1:A:655:GLY:HA2	1:A:658:LEU:HD12	2.02	0.41
1:B:169:LYS:C	1:B:173:ILE:HD13	2.40	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: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:868:GLU:C	1:A:870:ARG:H	2.28	0.40
1:B:489:ASP:O	1:B:490:ASP:HB2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:LYS:C	1:A:171:ASN:N	2.78	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:807:ASP:C	1:A:809:ASP:N	2.80	0.40
1:B:80:TRP:O	1:B:88:ARG:HD3	2.20	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:700:LEU:O	1:B:701:GLY:C	2.64	0.40
1:B:763:GLU:HA	1:B:766:LEU:HD12	2.03	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:B:509:LYS:O	1:B:513:THR:OG1	2.33	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: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%)	12	45
1	B	834/876 (95%)	712 (85%)	110 (13%)	12 (1%)	9	39
2	C	32/40 (80%)	27 (84%)	4 (12%)	1 (3%)	3	22
2	D	21/40 (52%)	16 (76%)	5 (24%)	0	100	100
All	All	1754/1832 (96%)	1516 (86%)	216 (12%)	22 (1%)	9	40

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 ⓘ

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%)	685 (92%)	61 (8%)	10	39
1	B	722/751 (96%)	640 (89%)	82 (11%)	5	24
2	C	35/39 (90%)	32 (91%)	3 (9%)	10	36
All	All	1503/1541 (98%)	1357 (90%)	146 (10%)	8	32

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	9	LYS
1	A	18	LEU
1	A	68	LYS
1	A	121	ILE
1	A	161	ILE
1	A	166	LEU
1	A	172	GLU
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	413	LEU
1	A	417	MET
1	A	426	ASP
1	A	454	GLN
1	A	474	PHE
1	A	497	TYR
1	A	524	LEU
1	A	525	ARG
1	A	532	LEU
1	A	535	ILE
1	A	563	GLN
1	A	576	GLN
1	A	580	LEU
1	A	624	VAL
1	A	625	GLN
1	A	626	GLU
1	A	634	THR
1	A	635	LEU
1	A	637	GLU
1	A	647	MET
1	A	654	LEU
1	A	665	GLN
1	A	673	LEU
1	A	681	LEU
1	A	682	GLN
1	A	685	ILE
1	A	686	ILE

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Mol	Chain	Res	Type
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
1	A	754	MET
1	A	755	VAL
1	A	756	ASP
1	A	772	ILE
1	A	781	GLU
1	A	782	ASN
1	A	797	ILE
1	A	821	LEU
1	A	855	THR
1	A	856	ASN
1	A	857	LYS
2	C	29	SER
2	C	40	GLN
2	C	61	HIS
1	B	5	THR
1	B	7	LEU
1	B	9	LYS
1	B	15	ARG
1	B	18	LEU
1	B	27	ARG
1	B	44	LEU
1	B	71	ASP
1	B	73	LYS
1	B	79	ARG
1	B	96	LEU
1	B	111	GLN
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	263	ILE
1	B	336	ASN
1	B	352	LEU

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Mol	Chain	Res	Type
1	B	378	PRO
1	B	400	SER
1	B	417	MET
1	B	423	VAL
1	B	465	ARG
1	B	497	TYR
1	B	521	GLN
1	B	532	LEU
1	B	563	GLN
1	B	580	LEU
1	B	618	THR
1	B	624	VAL
1	B	625	GLN
1	B	626	GLU
1	B	632	VAL
1	B	633	SER
1	B	634	THR
1	B	635	LEU
1	B	636	VAL
1	B	639	LEU
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	712	GLN
1	B	722	LEU
1	B	727	GLU
1	B	730	LYS
1	B	731	TYR
1	B	737	ASN
1	B	747	VAL
1	B	757	TYR
1	B	758	LEU
1	B	766	LEU

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Mol	Chain	Res	Type
1	B	780	GLN
1	B	786	ASP
1	B	787	VAL
1	B	788	MET
1	B	800	PHE
1	B	804	ILE
1	B	811	THR
1	B	825	LEU
1	B	829	PHE
1	B	834	LEU
1	B	838	GLU
1	B	848	THR
1	B	851	ARG
1	B	852	ARG
1	B	853	SER
1	B	854	LYS
1	B	859	LYS
1	B	872	LEU
1	B	873	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	159	GLN
1	A	165	GLN
1	A	179	GLN
1	A	240	ASN
1	A	278	GLN
1	A	320	GLN
1	A	343	ASN
1	A	366	HIS
1	A	377	ASN
1	A	408	GLN
1	A	454	GLN
1	A	521	GLN
1	A	523	ASN
1	A	538	ASN
1	A	559	GLN
1	A	578	ASN
1	A	581	GLN
1	A	589	GLN

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Mol	Chain	Res	Type
1	A	596	GLN
1	A	602	GLN
1	A	682	GLN
1	A	706	HIS
1	A	712	GLN
1	A	737	ASN
1	A	740	GLN
1	A	744	GLN
1	A	759	ASN
1	A	780	GLN
1	A	856	ASN
2	C	60	ASN
1	B	22	GLN
1	B	60	GLN
1	B	132	GLN
1	B	141	ASN
1	B	159	GLN
1	B	171	ASN
1	B	179	GLN
1	B	208	ASN
1	B	227	GLN
1	B	240	ASN
1	B	278	GLN
1	B	285	ASN
1	B	320	GLN
1	B	343	ASN
1	B	377	ASN
1	B	401	GLN
1	B	408	GLN
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

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Mol	Chain	Res	Type
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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	871/876 (99%)	0.12	37 (4%) 40 25	11, 51, 141, 200	1 (0%)
1	B	845/876 (96%)	0.95	134 (15%) 5 3	14, 102, 189, 199	0
2	C	36/40 (90%)	0.28	0 100 100	31, 63, 103, 133	0
2	D	23/40 (57%)	0.84	2 (8%) 16 11	58, 70, 82, 90	0
All	All	1775/1832 (96%)	0.53	173 (9%) 13 9	11, 67, 178, 200	1 (0%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	790	VAL	9.2
1	B	731	TYR	7.1
1	B	825	LEU	5.7
1	B	829	PHE	5.7
1	B	801	ILE	5.3
1	B	800	PHE	5.2
1	B	797	ILE	5.1
1	B	59	LEU	4.9
1	B	791	GLN	4.8
1	A	561	VAL	4.7
1	B	604	SER	4.7
1	B	217	PHE	4.5
1	B	758	LEU	4.4
1	B	811	THR	4.4
1	B	156	TYR	4.3
1	B	830	GLY	4.3
1	A	855	THR	4.2
1	B	713	ILE	4.1
1	B	794	VAL	4.0
1	A	864	TRP	4.0
1	B	828	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	680	ALA	3.9
1	B	798	LEU	3.9
1	B	145	HIS	3.9
1	A	866	THR	3.9
1	B	681	LEU	3.9
1	A	781	GLU	3.8
1	B	812	ASP	3.8
1	A	807	ASP	3.5
1	B	803	HIS	3.5
1	B	119	ALA	3.5
1	B	518	ASP	3.4
1	B	807	ASP	3.4
1	B	95	VAL	3.4
1	B	761	LEU	3.4
1	B	501	SER	3.3
1	A	559	GLN	3.3
2	D	62	ALA	3.3
1	B	45	ALA	3.3
1	B	729	LYS	3.3
1	B	118	CYS	3.2
1	A	865	ALA	3.2
1	B	67	SER	3.2
1	B	639	LEU	3.2
1	B	400	SER	3.2
1	B	137	VAL	3.1
1	B	551	THR	3.1
1	A	869	LEU	3.1
1	B	203	GLU	3.1
1	B	813	GLY	3.1
1	B	160	ASP	3.1
1	B	876	ALA	3.1
1	A	6	ILE	3.1
1	B	827	THR	3.0
1	A	868	GLU	3.0
1	A	872	LEU	3.0
1	B	789	LEU	3.0
1	A	401	GLN	3.0
1	B	757	TYR	3.0
1	B	607	VAL	3.0
1	A	682	GLN	3.0
1	B	548	GLN	3.0
1	B	822	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	572	SER	2.9
1	B	788	MET	2.9
1	B	705	VAL	2.9
1	B	717	PHE	2.9
1	B	693	MET	2.9
1	B	36	PHE	2.8
1	B	747	VAL	2.8
1	B	677	LEU	2.8
1	B	561	VAL	2.8
1	B	692	VAL	2.8
1	B	100	GLY	2.8
1	A	104	TYR	2.8
1	B	823	GLY	2.7
1	B	608	MET	2.7
1	A	737	ASN	2.7
1	B	508	GLN	2.7
1	B	121	ILE	2.7
1	B	517	PRO	2.7
1	B	775	GLY	2.6
1	B	358	CYS	2.6
1	B	104	TYR	2.6
1	A	779	ASP	2.6
1	B	161	ILE	2.6
1	B	712	GLN	2.6
1	B	577	PHE	2.6
1	A	301	ALA	2.6
1	B	112	CYS	2.6
1	B	728	PHE	2.6
1	A	562	LEU	2.6
1	B	673	LEU	2.6
1	B	16	LEU	2.5
1	B	204	PHE	2.5
1	B	826	CYS	2.5
1	B	824	ASP	2.5
1	B	696	LEU	2.5
1	B	846	LEU	2.5
1	B	114	ALA	2.5
1	B	340	ASP	2.5
1	B	809	ASP	2.5
1	B	787	VAL	2.5
1	B	804	ILE	2.5
1	A	162	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	678	CYS	2.4
1	A	782	ASN	2.4
1	B	629	LEU	2.4
1	B	134	VAL	2.4
1	B	735	VAL	2.4
1	B	213	SER	2.4
1	B	730	LYS	2.4
1	B	30	VAL	2.4
1	B	810	HIS	2.4
1	B	75	GLN	2.4
2	D	58	TYR	2.4
1	B	207	ALA	2.4
1	A	691	GLU	2.4
1	B	785	PRO	2.4
1	B	620	GLY	2.4
1	A	621	SER	2.4
1	B	621	SER	2.4
1	B	709	VAL	2.4
1	B	105	ARG	2.3
1	B	98	THR	2.3
1	B	646	TYR	2.3
1	B	792	PRO	2.3
1	A	444	ILE	2.3
1	A	306	PRO	2.3
1	A	738	THR	2.3
1	A	498	CYS	2.3
1	B	817	CYS	2.3
1	B	22	GLN	2.2
1	B	732	LEU	2.2
1	B	780	GLN	2.2
1	B	719	ASP	2.2
1	B	21	ALA	2.2
1	B	216	HIS	2.2
1	B	43	VAL	2.2
1	B	52	VAL	2.2
1	B	836	LEU	2.2
1	B	640	GLY	2.2
1	A	334	ASP	2.2
1	B	831	LYS	2.2
1	A	569	GLN	2.2
1	A	683	SER	2.2
1	B	588	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	821	LEU	2.2
1	B	143	THR	2.1
1	B	514	THR	2.1
1	B	603	ILE	2.1
1	B	521	GLN	2.1
1	A	876	ALA	2.1
1	B	63	ASN	2.1
1	B	850	GLY	2.1
1	A	124	ASN	2.1
1	B	795	GLU	2.1
1	A	853	SER	2.1
1	B	110	SER	2.1
1	B	209	PHE	2.1
1	A	552	LEU	2.1
1	A	784	HIS	2.1
1	B	647	MET	2.1
1	B	559	GLN	2.1
1	B	158	CYS	2.1
1	A	619	ALA	2.1
1	B	636	VAL	2.0
1	B	600	ALA	2.0
1	A	637	GLU	2.0
1	B	637	GLU	2.0
1	B	448	TYR	2.0
1	B	401	GLN	2.0
1	B	504	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.