



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:54 PM UTC

PDB ID : 3AOB / pdb_00003aob
Title : Structures of the multidrug exporter AcrB reveal a proximal multisite drug-binding pocket
Authors : Nakashima, R.; Sakurai, K.; Yamaguchi, A.
Deposited on : 2010-09-23
Resolution : 3.35 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

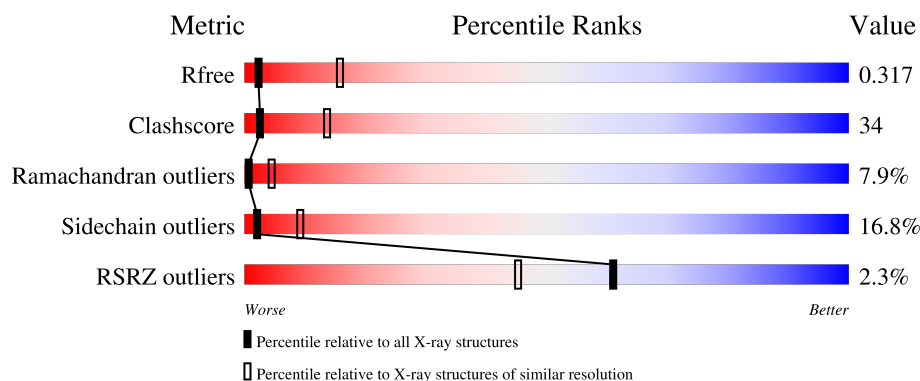
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	1053	2% 41% 43% 13% ..
1	B	1053	2% 35% 48% 14% .
1	C	1053	2% 39% 44% 12% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23385 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.

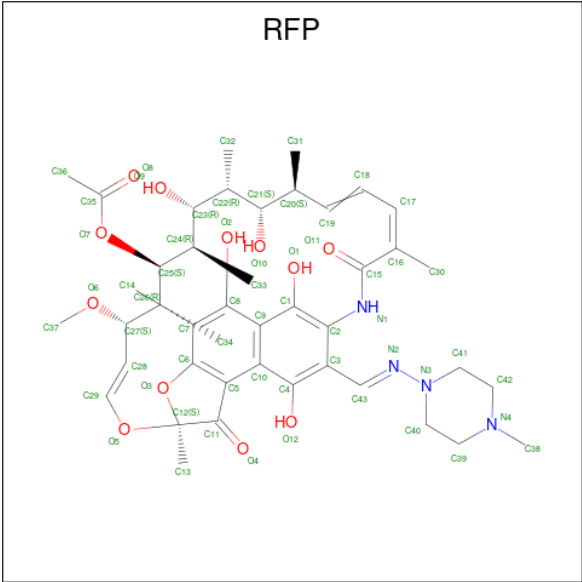
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
B	1051	HIS	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
C	1050	HIS	-	expression tag	UNP P31224
C	1051	HIS	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

- Molecule 2 is RIFAMPICIN (CCD ID: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			59	43	4	12		

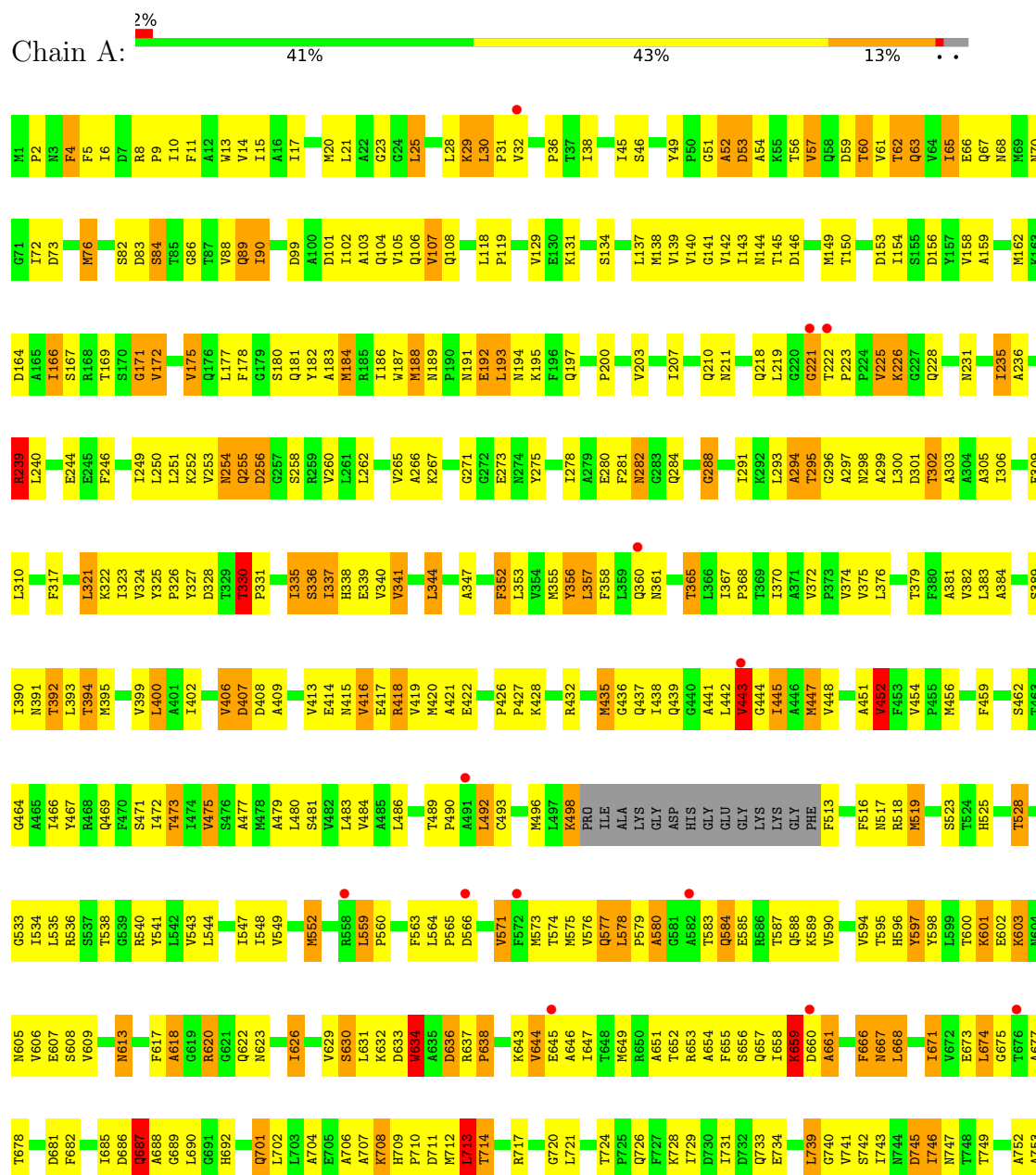
- Molecule 3 is water.

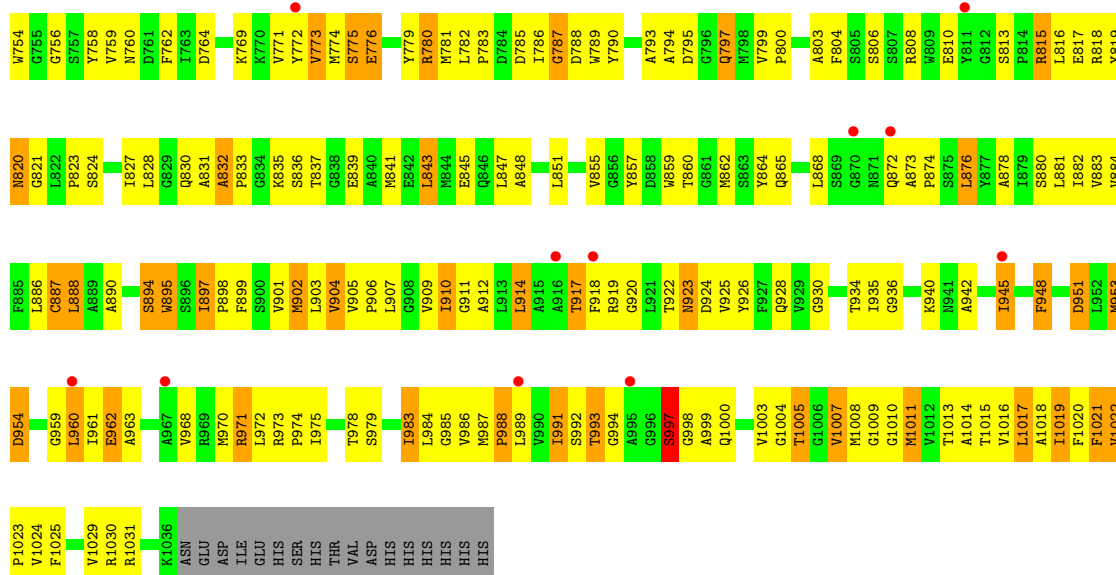
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0

3 Residue-property plots

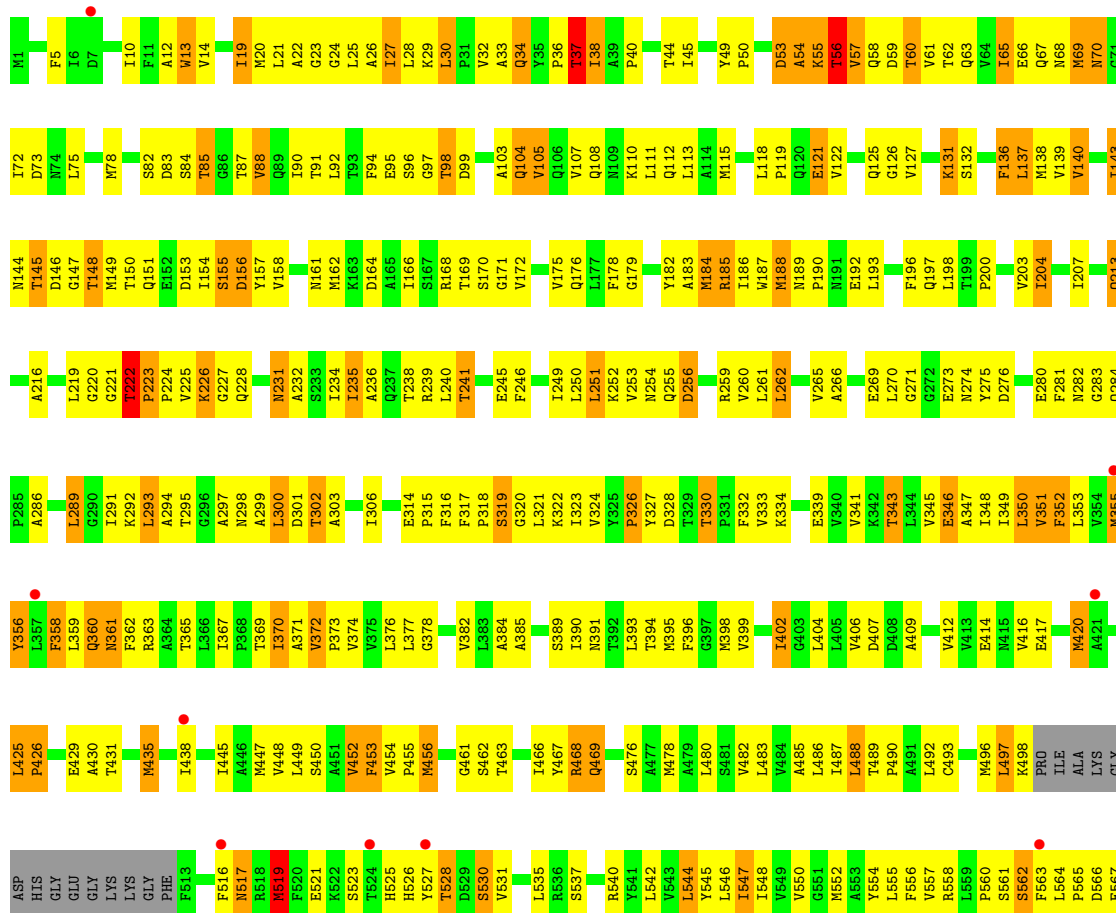
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

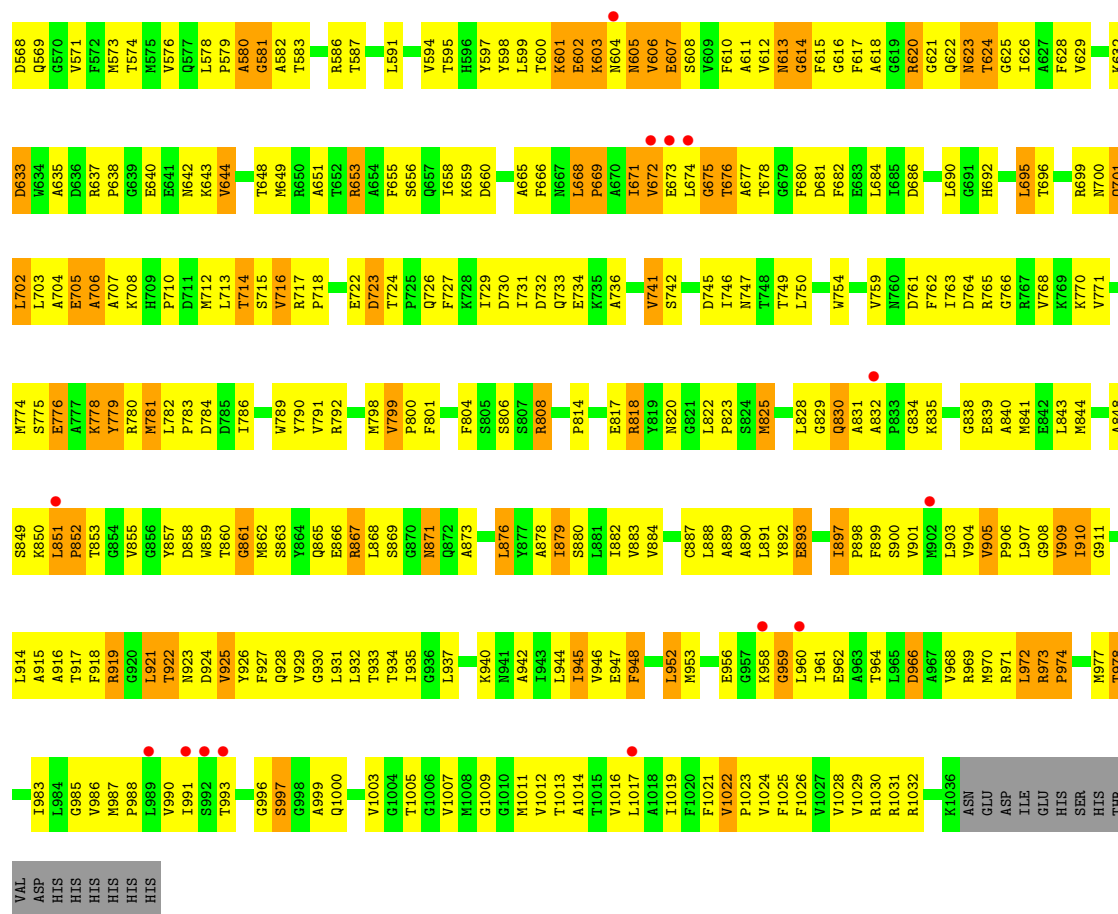
• Molecule 1: Acriflavine resistance protein B



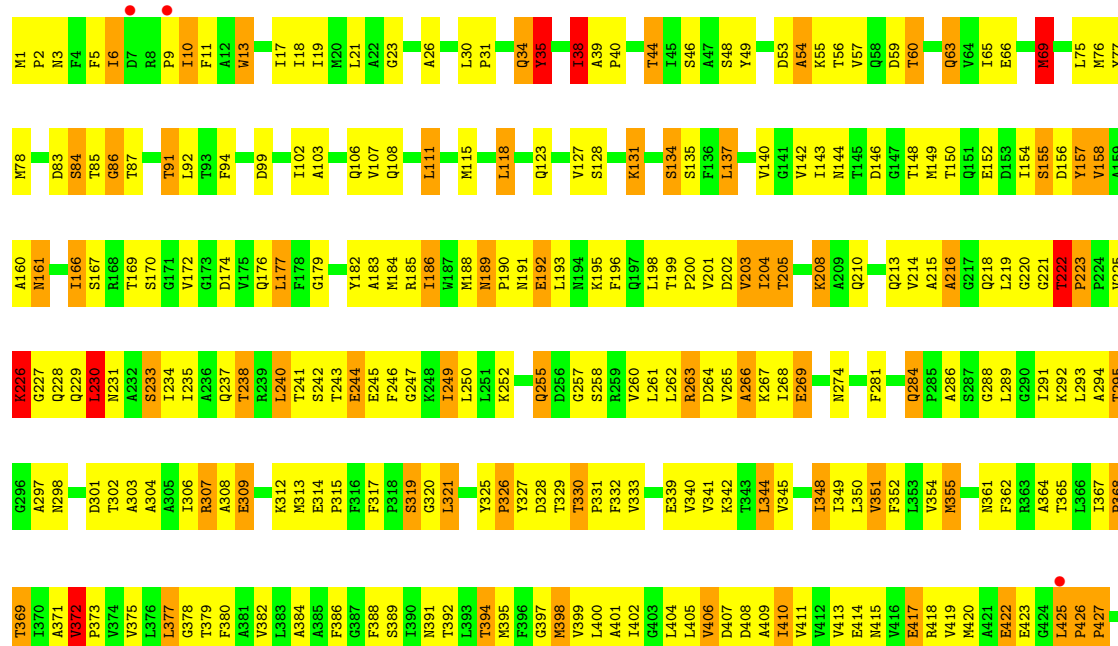


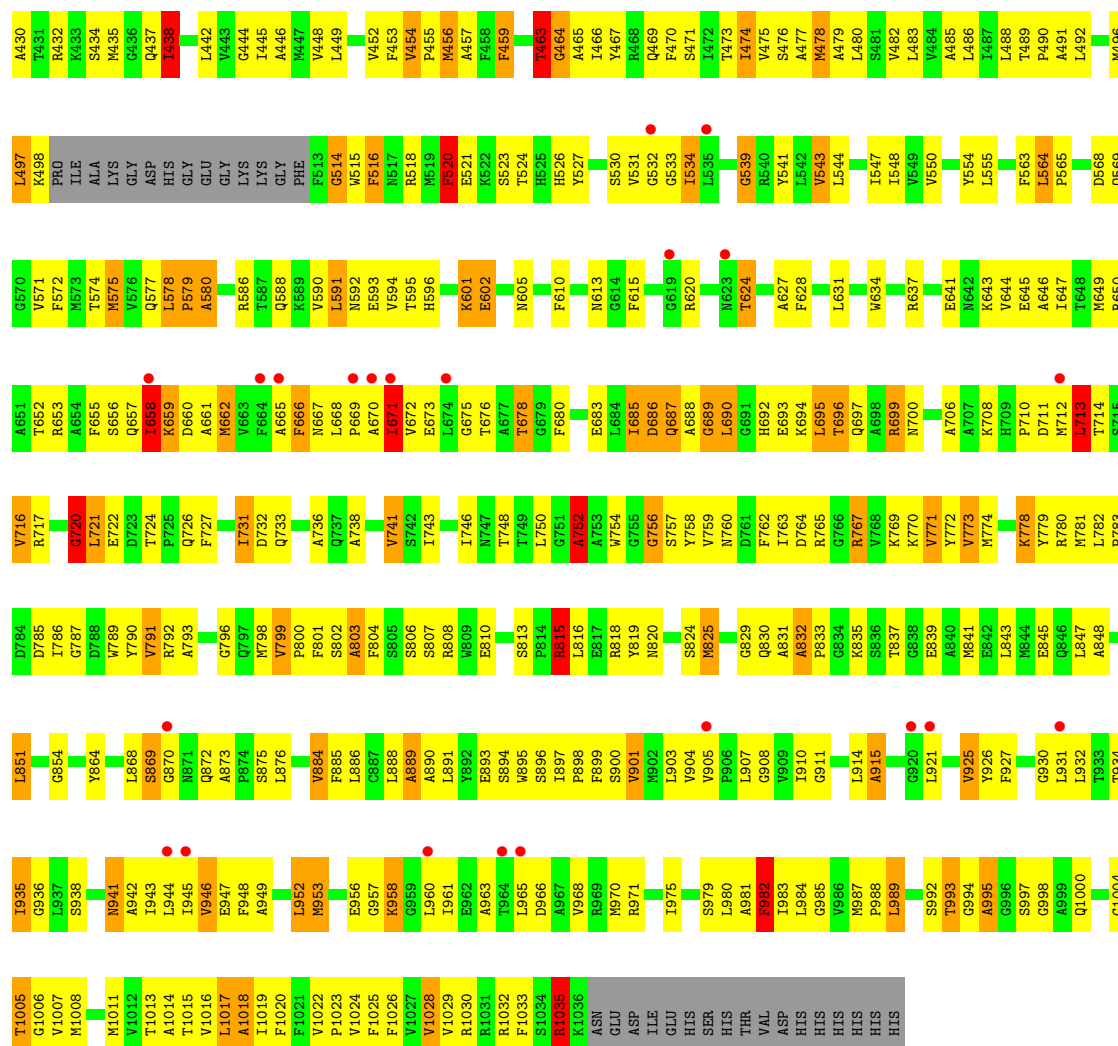
• Molecule 1: Acriflavine resistance protein B





• Molecule 1: Acriflavine resistance protein B





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.90Å 134.31Å 161.77Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	48.91 – 3.35 48.91 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.91-3.35) 97.6 (48.91-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.64 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.261 , 0.326 0.256 , 0.317	Depositor DCC
R_{free} test set	3350 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23385	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

Bond lengths and bond angles in the following residue types are not validated in this section: RFP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.81	2/7920 (0.0%)	1.07	19/10756 (0.2%)
1	B	0.77	2/7920 (0.0%)	1.11	35/10756 (0.3%)
1	C	0.81	4/7920 (0.1%)	1.11	25/10756 (0.2%)
All	All	0.80	8/23760 (0.0%)	1.10	79/32268 (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	C	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	905	VAL	CA-CB	7.57	1.57	1.54
1	A	372	VAL	CA-CB	6.84	1.58	1.54
1	C	330	THR	CA-CB	5.83	1.59	1.54
1	A	1022	VAL	CA-CB	5.74	1.57	1.53
1	C	671	ILE	CA-CB	5.26	1.61	1.54
1	C	203	VAL	CA-CB	-5.15	1.48	1.54
1	C	38	ILE	CA-CB	5.11	1.61	1.54
1	B	672	VAL	CA-CB	5.08	1.61	1.54

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	TYR	N-CA-CB	-12.98	88.53	110.33
1	B	355	MET	CB-CA-C	12.68	132.23	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	LEU	CA-C-N	8.52	129.15	120.38
1	B	425	LEU	C-N-CA	8.52	129.15	120.38
1	B	55	LYS	N-CA-C	-8.25	101.34	111.40
1	C	161	ASN	N-CA-C	8.05	124.02	114.04
1	C	309	GLU	N-CA-C	-7.58	102.95	111.14
1	B	25	LEU	N-CA-C	-7.54	103.00	111.07
1	B	426	PRO	N-CA-C	7.40	119.73	110.70
1	C	166	ILE	N-CA-C	-7.22	103.25	110.62
1	B	352	PHE	CB-CA-C	7.11	122.65	110.84
1	B	353	LEU	N-CA-C	6.95	119.45	111.11
1	C	660	ASP	N-CA-C	-6.91	106.05	114.75
1	C	286	ALA	N-CA-C	6.77	116.93	108.19
1	B	830	GLN	N-CA-C	6.76	116.92	108.19
1	C	752	ALA	N-CA-C	-6.70	96.53	110.80
1	C	35	TYR	CA-C-N	-6.63	111.55	119.84
1	C	35	TYR	C-N-CA	-6.63	111.55	119.84
1	C	799	VAL	N-CA-C	6.61	114.31	108.63
1	C	426	PRO	N-CA-C	6.45	118.57	110.70
1	B	799	VAL	N-CA-C	6.37	115.56	108.05
1	A	644	VAL	N-CA-C	6.35	117.28	111.81
1	B	799	VAL	CA-C-N	6.19	126.13	119.76
1	B	799	VAL	C-N-CA	6.19	126.13	119.76
1	A	1021	PHE	N-CA-C	6.18	118.09	111.36
1	B	409	ALA	N-CA-C	-6.16	106.40	114.04
1	B	832	ALA	CA-C-N	-6.09	113.47	120.04
1	B	832	ALA	C-N-CA	-6.09	113.47	120.04
1	B	822	LEU	CA-C-N	6.06	125.82	119.76
1	B	822	LEU	C-N-CA	6.06	125.82	119.76
1	C	157	TYR	N-CA-C	-5.94	103.77	111.02
1	A	1009	GLY	N-CA-C	-5.94	105.10	111.93
1	B	148	THR	N-CA-C	-5.94	105.69	113.17
1	B	273	GLU	N-CA-C	-5.92	104.41	111.69
1	A	559	LEU	CA-C-N	5.91	125.85	119.76
1	A	559	LEU	C-N-CA	5.91	125.85	119.76
1	C	864	TYR	N-CA-C	-5.87	105.96	114.12
1	B	207	ILE	CB-CA-C	-5.86	104.35	112.02
1	C	474	ILE	N-CA-C	5.83	116.61	110.72
1	A	953	MET	N-CA-C	-5.82	107.42	114.75
1	A	797	GLN	N-CA-C	5.78	118.37	109.07
1	A	954	ASP	N-CA-C	-5.73	106.83	113.88
1	C	1033	PHE	N-CA-C	5.71	117.85	110.65
1	B	115	MET	N-CA-C	5.71	122.43	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ARG	N-CA-C	5.69	122.91	110.80
1	B	32	VAL	CB-CA-C	-5.63	102.81	110.42
1	A	601	LYS	N-CA-C	-5.63	106.45	113.15
1	A	878	ALA	N-CA-C	-5.61	104.86	110.97
1	B	221	GLY	N-CA-C	5.61	119.52	112.79
1	C	720	GLY	N-CA-C	5.60	126.45	113.18
1	A	894	SER	N-CA-C	5.59	118.21	108.76
1	C	666	PHE	N-CA-C	5.57	116.73	108.60
1	A	418	ARG	N-CA-C	-5.54	105.31	112.68
1	C	127	VAL	N-CA-C	-5.53	103.96	110.21
1	B	666	PHE	N-CA-C	5.50	118.65	109.96
1	B	528	THR	N-CA-C	-5.46	106.68	113.55
1	C	960	LEU	N-CA-C	5.46	117.66	111.11
1	B	38	ILE	CB-CA-C	-5.45	107.08	111.71
1	B	303	ALA	N-CA-C	-5.40	105.81	112.72
1	C	810	GLU	N-CA-C	5.37	116.38	107.73
1	B	85	THR	N-CA-C	-5.37	107.38	114.31
1	A	713	LEU	N-CA-C	5.35	122.20	110.80
1	B	40	PRO	O-C-N	5.29	123.74	121.31
1	A	573	MET	N-CA-C	5.26	117.75	108.75
1	B	131	LYS	N-CA-C	-5.25	102.50	110.28
1	C	321	LEU	CA-CB-CG	5.19	134.48	116.30
1	C	426	PRO	CA-C-N	5.17	126.31	119.84
1	C	426	PRO	C-N-CA	5.17	126.31	119.84
1	C	157	TYR	N-CA-CB	5.16	117.66	109.82
1	A	45	ILE	CB-CA-C	-5.15	104.46	111.15
1	A	820	ASN	N-CA-C	5.14	118.29	111.30
1	A	897	ILE	N-CA-CB	5.12	113.95	110.52
1	B	88	VAL	N-CA-C	5.10	116.06	108.46
1	C	214	VAL	CB-CA-C	-5.10	104.10	111.34
1	A	687	GLN	N-CA-C	5.07	119.15	112.92
1	B	701	GLN	N-CA-C	-5.03	107.42	113.21
1	B	175	VAL	N-CA-C	5.02	115.20	107.77
1	C	1035	ARG	N-CA-C	5.02	117.48	109.96
1	B	487	ILE	N-CA-C	-5.01	107.66	111.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	221	GLY	Peptide
1	C	222	THR	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	7774	0	7931	501	0
1	B	7774	0	7931	572	0
1	C	7774	0	7931	605	0
2	C	59	0	57	10	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	23385	0	23850	1623	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 34.

All (1623) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:MET:HB3	1:A:887:CYS:SG	1.82	1.20
1:C:222:THR:HG23	1:C:223:PRO:CD	1.73	1.17
1:C:815:ARG:HG2	1:C:815:ARG:HH11	1.09	1.17
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.31	1.12
1:A:379:THR:HG21	1:A:477:ALA:HA	1.27	1.12
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.32	1.11
1:C:355:MET:HE3	1:C:355:MET:HA	1.35	1.07
1:C:222:THR:HG23	1:C:223:PRO:HD2	1.07	1.06
1:A:275:TYR:HB3	1:C:223:PRO:HD3	1.38	1.06
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.29	1.05
1:B:367:ILE:HG13	1:B:492:LEU:HB3	1.37	1.03
1:C:564:LEU:HD13	1:C:671:ILE:HD12	1.38	1.01
1:B:219:LEU:HG	1:B:234:ILE:HD11	1.40	0.99
1:C:188:MET:HE1	1:C:200:PRO:HA	1.45	0.99
1:C:222:THR:CG2	1:C:223:PRO:HD2	1.93	0.99
1:B:860:THR:HG22	1:B:861:GLY:H	1.24	0.99
1:A:400:LEU:HD11	1:A:930:GLY:HA2	1.41	0.98
1:A:414:GLU:HG2	1:A:974:PRO:HG3	1.47	0.97
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.44	0.97
1:B:95:GLU:O	1:B:98:THR:HG22	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.48	0.95
1:B:222:THR:HB	1:B:223:PRO:CD	1.95	0.95
1:A:167:SER:OG	1:A:175:VAL:HG21	1.64	0.95
1:B:65:ILE:HG22	1:B:69:MET:HE1	1.48	0.94
1:A:674:LEU:HD22	1:A:675:GLY:H	1.33	0.93
1:C:367:ILE:HD11	1:C:492:LEU:HB3	1.50	0.93
1:C:911:GLY:HA3	1:C:1013:THR:HG21	1.47	0.93
1:C:832:ALA:HB3	1:C:833:PRO:HD3	1.49	0.92
1:C:267:LYS:HE3	1:C:269:GLU:HG2	1.52	0.92
1:A:713:LEU:HD23	1:A:833:PRO:HD3	1.50	0.92
1:B:255:GLN:HG3	1:B:256:ASP:OD1	1.70	0.91
1:C:372:VAL:HG12	1:C:373:PRO:HD3	1.50	0.91
1:A:221:GLY:HA2	1:B:622:GLN:NE2	1.86	0.91
1:A:383:LEU:HD21	1:A:473:THR:HG23	1.53	0.90
1:A:407:ASP:OD2	1:A:978:THR:HG21	1.71	0.90
1:B:136:PHE:HE1	1:B:617:PHE:CZ	1.90	0.90
1:C:146:ASP:CB	1:C:148:THR:HG23	2.01	0.90
1:B:222:THR:HB	1:B:223:PRO:HD3	1.53	0.90
1:B:225:VAL:H	1:C:781:MET:HE3	1.33	0.90
1:A:634:TRP:H	1:A:634:TRP:CD1	1.89	0.89
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.55	0.89
1:A:221:GLY:HA2	1:B:622:GLN:HE22	1.37	0.89
1:A:901:VAL:O	1:A:904:VAL:HG23	1.74	0.88
1:A:993:THR:HB	1:A:997:SER:HB3	1.54	0.88
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.54	0.88
1:B:355:MET:O	1:B:359:LEU:CB	2.22	0.88
1:C:55:LYS:HE2	1:C:59:ASP:OD1	1.74	0.88
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.36	0.88
1:A:275:TYR:CB	1:C:223:PRO:HD3	2.02	0.88
1:B:463:THR:HG21	1:B:869:SER:HB2	1.56	0.87
1:B:867:ARG:HG2	1:B:868:LEU:HD22	1.57	0.87
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.54	0.87
1:C:713:LEU:HD23	1:C:831:ALA:HA	1.57	0.86
1:B:876:LEU:O	1:B:880:SER:HB2	1.74	0.86
1:C:815:ARG:HG2	1:C:815:ARG:NH1	1.90	0.86
1:A:552:MET:HE1	1:A:906:PRO:HB3	1.58	0.85
1:C:146:ASP:HB3	1:C:148:THR:CG2	2.05	0.85
1:B:139:VAL:HG12	1:B:139:VAL:O	1.74	0.85
1:C:345:VAL:O	1:C:348:ILE:HG22	1.76	0.85
1:C:131:LYS:HB2	1:C:295:THR:HG21	1.59	0.84
1:C:246:PHE:O	1:C:249:ILE:HG13	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:911:GLY:HA3	1:C:1013:THR:CG2	2.07	0.84
1:C:53:ASP:O	1:C:84:SER:HA	1.75	0.84
1:C:968:VAL:HG11	1:C:1023:PRO:HG3	1.57	0.84
1:B:225:VAL:HG22	1:C:781:MET:HE3	1.59	0.84
1:B:918:PHE:HD1	1:B:919:ARG:HD3	1.41	0.84
1:C:953:MET:SD	1:C:963:ALA:HB2	2.18	0.84
1:B:200:PRO:HD2	1:B:749:THR:CG2	2.08	0.84
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.13	0.84
1:B:171:GLY:HA3	1:B:302:THR:HB	1.59	0.84
1:B:729:ILE:HG13	1:B:730:ASP:H	1.44	0.83
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.58	0.83
1:B:274:ASN:HD22	1:B:276:ASP:HB2	1.43	0.83
1:C:131:LYS:HB2	1:C:295:THR:CG2	2.09	0.82
1:B:835:LYS:HB2	1:B:839:GLU:OE2	1.77	0.82
1:B:226:LYS:NZ	1:B:226:LYS:HA	1.95	0.82
1:B:552:MET:SD	1:B:909:VAL:HG23	2.20	0.81
1:A:961:ILE:HD11	1:A:1031:ARG:NH1	1.95	0.81
1:B:892:TYR:HB2	1:B:897:ILE:HD11	1.61	0.81
1:C:375:VAL:HG11	1:C:405:LEU:HD22	1.61	0.81
1:A:389:SER:O	1:A:394:THR:HG21	1.80	0.81
1:B:355:MET:O	1:B:359:LEU:HB2	1.80	0.81
1:C:889:ALA:HB2	1:C:898:PRO:HG3	1.61	0.81
1:A:60:THR:HG23	1:A:119:PRO:HG3	1.62	0.81
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.61	0.81
1:A:993:THR:HG21	1:A:1000:GLN:OE1	1.80	0.81
1:C:568:ASP:OD2	1:C:644:VAL:HG23	1.80	0.81
1:A:180:SER:O	1:A:181:GLN:HB3	1.81	0.81
1:A:728:LYS:HD3	1:C:235:ILE:HG22	1.62	0.81
1:B:298:ASN:HB2	1:B:301:ASP:HB2	1.62	0.80
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.63	0.80
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.10	0.80
1:B:94:PHE:HB3	1:B:98:THR:HG21	1.62	0.80
1:B:226:LYS:HA	1:B:226:LYS:HZ3	1.46	0.80
1:C:190:PRO:HD2	1:C:779:TYR:CD1	2.17	0.80
1:A:435:MET:HE2	1:A:438:ILE:HD11	1.63	0.80
1:A:713:LEU:HD12	1:A:830:GLN:HB2	1.64	0.79
1:B:435:MET:HE3	1:B:435:MET:HA	1.63	0.79
1:C:31:PRO:O	1:C:389:SER:HB2	1.81	0.79
1:C:355:MET:HA	1:C:355:MET:CE	2.10	0.79
1:C:459:PHE:HD1	1:C:459:PHE:N	1.81	0.79
1:B:72:ILE:HD11	1:B:110:LYS:HG3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.63	0.79
1:A:379:THR:CG2	1:A:477:ALA:HA	2.09	0.79
1:A:108:GLN:NE2	1:B:112:GLN:HB3	1.97	0.79
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.63	0.79
1:A:267:LYS:HE2	1:A:776:GLU:OE2	1.83	0.79
1:B:668:LEU:HB3	1:B:676:THR:HG23	1.65	0.78
1:A:375:VAL:O	1:A:379:THR:HG23	1.83	0.78
1:B:250:LEU:HD12	1:B:259:ARG:HH21	1.48	0.78
1:C:355:MET:SD	1:C:410:ILE:HD11	2.23	0.78
1:B:23:GLY:HA3	1:B:377:LEU:O	1.83	0.78
1:B:1026:PHE:O	1:B:1030:ARG:HB2	1.83	0.78
1:B:905:VAL:HG13	1:B:906:PRO:HD3	1.63	0.77
1:A:923:ASN:C	1:A:923:ASN:HD22	1.92	0.77
1:A:437:GLN:HB3	1:A:948:PHE:HE2	1.50	0.77
1:C:246:PHE:O	1:C:249:ILE:CG1	2.32	0.77
1:A:720:GLY:O	1:A:721:LEU:HD23	1.85	0.77
1:B:224:PRO:HA	1:C:781:MET:HE1	1.66	0.77
1:B:919:ARG:HG3	1:B:1005:THR:HG21	1.67	0.77
1:C:945:ILE:C	1:C:947:GLU:H	1.93	0.77
1:B:910:ILE:O	1:B:914:LEU:HB2	1.84	0.76
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.15	0.76
1:B:416:VAL:CG2	1:B:431:THR:HA	2.15	0.76
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.66	0.76
1:C:186:ILE:HG12	1:C:262:LEU:HD21	1.68	0.76
1:C:767:ARG:HH11	1:C:767:ARG:HG3	1.49	0.76
1:B:394:THR:HG23	1:B:469:GLN:HG3	1.68	0.76
1:C:662:MET:HE2	1:C:662:MET:H	1.49	0.76
1:A:418:ARG:HH12	1:A:973:ARG:HB3	1.49	0.76
1:A:56:THR:O	1:A:60:THR:HB	1.85	0.76
1:A:781:MET:HE3	1:C:228:GLN:OE1	1.86	0.76
1:A:961:ILE:HD11	1:A:1031:ARG:HH12	1.51	0.76
1:B:327:TYR:HB2	1:B:628:PHE:HB3	1.68	0.76
1:B:360:GLN:O	1:B:361:ASN:HB3	1.86	0.76
1:A:52:ALA:HB3	1:A:86:GLY:HA2	1.68	0.75
1:C:188:MET:HE2	1:C:193:LEU:HD11	1.68	0.75
1:A:435:MET:SD	1:A:490:PRO:HB3	2.26	0.75
1:A:733:GLN:HE21	1:C:210:GLN:HG2	1.50	0.75
1:B:1021:PHE:O	1:B:1024:VAL:HB	1.86	0.75
1:A:13:TRP:O	1:A:17:ILE:HG13	1.86	0.75
1:C:712:MET:O	1:C:714:THR:HG23	1.85	0.75
1:B:574:THR:HG23	1:B:665:ALA:HB2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLN:H	1:C:34:GLN:HE21	1.35	0.74
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.68	0.74
1:C:459:PHE:N	1:C:459:PHE:CD1	2.54	0.74
1:B:722:GLU:O	1:B:723:ASP:O	2.04	0.74
1:B:10:ILE:HD12	1:C:893:GLU:O	1.86	0.74
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.68	0.74
1:C:242:SER:HB3	1:C:245:GLU:HG3	1.70	0.74
1:C:767:ARG:HH11	1:C:767:ARG:CG	1.99	0.74
1:A:464:GLY:HA2	1:A:467:TYR:HB2	1.69	0.74
1:B:314:GLU:HG2	1:B:317:PHE:CE2	2.23	0.74
1:A:73:ASP:H	1:A:106:GLN:HE22	1.36	0.74
1:B:241:THR:HG22	1:B:763:ILE:O	1.88	0.74
1:B:699:ARG:HH11	1:B:699:ARG:HB3	1.52	0.74
1:C:202:ASP:OD2	1:C:792:ARG:NH2	2.21	0.74
1:A:14:VAL:HG21	1:B:890:ALA:HB2	1.70	0.73
1:A:574:THR:HG21	1:A:594:VAL:HG11	1.69	0.73
1:C:953:MET:HE1	1:C:1030:ARG:HE	1.53	0.73
1:C:414:GLU:HA	1:C:417:GLU:HG2	1.67	0.73
1:C:575:MET:SD	1:C:575:MET:N	2.61	0.73
1:B:185:ARG:HH11	1:B:185:ARG:CG	2.01	0.73
1:B:26:ALA:O	1:B:30:LEU:HB2	1.88	0.73
1:B:730:ASP:HB3	1:B:806:SER:HB3	1.71	0.73
1:B:355:MET:O	1:B:359:LEU:HB3	1.88	0.73
1:B:370:ILE:HG22	1:B:370:ILE:O	1.87	0.73
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.71	0.73
1:A:317:PHE:HB3	1:A:321:LEU:CD2	2.17	0.73
1:C:345:VAL:O	1:C:348:ILE:CG2	2.37	0.73
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.89	0.73
1:C:792:ARG:HB2	1:C:798:MET:HE1	1.69	0.73
1:B:188:MET:HB2	1:B:775:SER:HA	1.70	0.73
1:C:425:LEU:HB2	1:C:426:PRO:HD3	1.70	0.73
1:A:2:PRO:O	1:A:6:ILE:HG23	1.89	0.72
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.24	0.72
1:A:945:ILE:HG13	1:A:971:ARG:HG2	1.71	0.72
1:A:447:MET:CB	1:A:887:CYS:SG	2.72	0.72
1:A:101:ASP:O	1:A:105:VAL:HG23	1.88	0.72
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.19	0.72
1:A:471:SER:O	1:A:475:VAL:HG12	1.87	0.72
1:B:274:ASN:ND2	1:B:276:ASP:HB2	2.03	0.72
1:C:983:ILE:HG23	1:C:1008:MET:HG3	1.69	0.72
1:B:452:VAL:O	1:B:453:PHE:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:MET:HB2	1:C:498:LYS:HE2	1.71	0.72
1:A:4:PHE:O	1:A:8:ARG:NH2	2.23	0.72
1:B:706:ALA:C	1:B:708:LYS:H	1.97	0.72
1:C:463:THR:HG23	1:C:563:PHE:HE1	1.54	0.72
1:A:613:ASN:C	1:A:613:ASN:HD22	1.98	0.71
1:B:399:VAL:O	1:B:402:ILE:HG22	1.89	0.71
1:B:416:VAL:HG22	1:B:431:THR:HA	1.72	0.71
1:C:643:LYS:O	1:C:647:ILE:HG12	1.88	0.71
1:B:197:GLN:O	1:B:792:ARG:NH2	2.22	0.71
1:C:832:ALA:CB	1:C:833:PRO:HD3	2.21	0.71
1:A:375:VAL:HG21	1:A:481:SER:HA	1.73	0.71
1:C:456:MET:HA	1:C:459:PHE:CE1	2.25	0.71
1:C:456:MET:HA	1:C:459:PHE:HE1	1.55	0.71
1:C:694:LYS:O	1:C:697:GLN:HB2	1.91	0.71
1:C:5:PHE:HE2	1:C:11:PHE:CD2	2.08	0.71
1:C:350:LEU:HD12	1:C:985:GLY:HA2	1.73	0.71
1:A:139:VAL:HG12	1:A:327:TYR:CB	2.21	0.71
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.71	0.71
1:C:815:ARG:HH11	1:C:815:ARG:CG	1.94	0.71
1:C:351:VAL:HG13	1:C:981:ALA:HB1	1.73	0.71
1:B:136:PHE:CE1	1:B:617:PHE:CZ	2.77	0.71
1:B:328:ASP:OD2	1:B:330:THR:HG22	1.90	0.71
1:A:707:ALA:O	1:A:710:PRO:HD3	1.91	0.70
1:B:171:GLY:HA3	1:B:302:THR:CB	2.20	0.70
1:B:412:VAL:HG13	1:B:435:MET:HE1	1.73	0.70
1:B:36:PRO:O	1:B:38:ILE:HG12	1.90	0.70
1:B:734:GLU:C	1:B:736:ALA:H	1.99	0.70
1:B:970:MET:HE2	1:B:970:MET:HA	1.73	0.70
1:B:188:MET:HE1	1:B:203:VAL:HG21	1.71	0.70
1:C:534:ILE:O	1:C:539:GLY:HA3	1.90	0.70
1:A:383:LEU:HD21	1:A:473:THR:CG2	2.20	0.70
1:B:911:GLY:HA3	1:B:1013:THR:HG21	1.74	0.70
1:C:601:LYS:O	1:C:602:GLU:HG2	1.91	0.70
1:A:337:ILE:HD11	1:A:395:MET:HG3	1.73	0.70
1:A:707:ALA:C	1:A:709:HIS:H	1.97	0.70
1:C:713:LEU:HD22	1:C:713:LEU:O	1.92	0.70
1:C:713:LEU:HD23	1:C:830:GLN:O	1.91	0.70
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.26	0.70
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.22	0.70
1:C:1:MET:HB2	1:C:2:PRO:CD	2.22	0.70
1:C:379:THR:HG21	1:C:398:MET:HE1	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:952:LEU:HA	1:C:956:GLU:HB3	1.73	0.70
1:B:445:ILE:HG23	1:B:940:LYS:HG3	1.74	0.69
1:C:911:GLY:CA	1:C:1013:THR:HG21	2.21	0.69
1:C:265:VAL:O	1:C:265:VAL:HG23	1.92	0.69
1:A:360:GLN:HB2	1:A:513:PHE:HB2	1.72	0.69
1:A:418:ARG:NH1	1:A:973:ARG:HB3	2.06	0.69
1:C:65:ILE:HD13	1:C:111:LEU:HD21	1.73	0.69
1:B:851:LEU:N	1:B:852:PRO:HD3	2.08	0.69
1:A:552:MET:HE1	1:A:906:PRO:CB	2.23	0.69
1:B:291:ILE:HG21	1:B:306:ILE:CD1	2.23	0.69
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.23	0.69
1:B:68:ASN:O	1:B:110:LYS:HE3	1.93	0.69
1:B:780:ARG:O	1:B:781:MET:HE2	1.91	0.69
1:C:722:GLU:OE1	1:C:722:GLU:HA	1.91	0.69
2:C:2002:RFP:H311	2:C:2002:RFP:H323	1.75	0.69
1:B:231:ASN:C	1:B:231:ASN:ND2	2.51	0.69
1:C:380:PHE:CE1	1:C:398:MET:SD	2.86	0.69
1:A:781:MET:HE3	1:C:228:GLN:CD	2.18	0.69
1:A:888:LEU:HB3	1:A:898:PRO:HB3	1.75	0.69
1:C:155:SER:OG	1:C:179:GLY:HA3	1.93	0.69
1:A:753:ALA:O	1:A:775:SER:HB3	1.94	0.68
1:B:860:THR:HG22	1:B:861:GLY:N	2.03	0.68
1:A:658:ILE:HG22	1:A:659:LYS:HD2	1.74	0.68
1:C:756:GLY:CA	1:C:774:MET:HG3	2.23	0.68
1:C:762:PHE:CE2	1:C:764:ASP:HB2	2.29	0.68
1:C:34:GLN:HG3	1:C:333:VAL:HG11	1.74	0.68
1:C:956:GLU:CD	1:C:957:GLY:H	2.00	0.68
1:A:597:TYR:CD1	1:A:597:TYR:C	2.71	0.68
1:B:680:PHE:HD1	1:B:859:TRP:HZ3	1.41	0.68
1:B:699:ARG:HB3	1:B:699:ARG:NH1	2.09	0.68
1:B:937:LEU:HD22	1:B:1011:MET:HE2	1.75	0.68
1:C:523:SER:HA	1:C:526:HIS:HB2	1.75	0.68
1:A:579:PRO:HG3	1:A:660:ASP:HB2	1.75	0.68
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.28	0.68
1:B:136:PHE:CE1	1:B:617:PHE:HZ	2.12	0.68
1:B:372:VAL:HB	1:B:402:ILE:HD11	1.76	0.68
1:A:51:GLY:O	1:C:215:ALA:HB1	1.93	0.68
1:B:1024:VAL:O	1:B:1028:VAL:HG23	1.94	0.68
1:C:244:GLU:HA	1:C:263:ARG:NH2	2.09	0.68
1:C:459:PHE:HD1	1:C:459:PHE:H	1.42	0.68
1:B:84:SER:HB3	1:B:814:PRO:HA	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HH22	1:B:774:MET:HE2	1.57	0.67
1:B:222:THR:CB	1:B:223:PRO:HD3	2.23	0.67
1:C:406:VAL:C	1:C:408:ASP:H	2.02	0.67
1:A:924:ASP:O	1:A:928:GLN:HG3	1.94	0.67
1:B:314:GLU:HG2	1:B:317:PHE:HE2	1.56	0.67
1:B:252:LYS:HB3	1:B:260:VAL:HG12	1.76	0.67
1:C:476:SER:O	1:C:477:ALA:HB3	1.94	0.67
1:A:418:ARG:HH12	1:A:973:ARG:CB	2.08	0.67
1:B:343:THR:HG21	1:B:1000:GLN:OE1	1.93	0.67
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.24	0.67
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.30	0.67
1:A:1025:PHE:O	1:A:1029:VAL:HG23	1.95	0.67
1:A:138:MET:HB2	1:A:327:TYR:O	1.95	0.67
1:B:14:VAL:HG21	1:C:890:ALA:HB2	1.77	0.67
1:C:824:SER:OG	1:C:825:MET:N	2.26	0.67
1:B:298:ASN:CB	1:B:301:ASP:HB2	2.25	0.67
1:B:778:LYS:H	1:B:778:LYS:HD3	1.59	0.67
1:C:56:THR:O	1:C:60:THR:HB	1.93	0.67
1:C:210:GLN:HE22	1:C:250:LEU:H	1.42	0.67
1:C:339:GLU:OE2	1:C:995:ALA:HB3	1.95	0.67
1:A:795:ASP:OD1	1:A:797:GLN:HG2	1.95	0.66
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.61	0.66
1:A:880:SER:O	1:A:884:VAL:HG23	1.94	0.66
1:C:200:PRO:O	1:C:204:ILE:HG12	1.95	0.66
1:C:521:GLU:HA	1:C:524:THR:OG1	1.95	0.66
1:B:961:ILE:HD11	1:B:1031:ARG:HH12	1.60	0.66
1:C:355:MET:HB3	1:C:365:THR:HG23	1.77	0.66
1:B:778:LYS:C	1:B:780:ARG:H	2.04	0.66
1:C:824:SER:O	1:C:825:MET:HB2	1.95	0.66
1:B:860:THR:CG2	1:B:861:GLY:H	2.05	0.66
1:A:1029:VAL:HG12	1:A:1030:ARG:H	1.60	0.66
1:B:144:ASN:HD21	1:B:148:THR:H	1.44	0.66
1:B:736:ALA:HB1	1:B:741:VAL:HG12	1.77	0.66
1:B:880:SER:O	1:B:884:VAL:HG23	1.96	0.66
1:C:252:LYS:O	1:C:260:VAL:HG12	1.95	0.66
1:A:188:MET:HA	1:A:266:ALA:HB2	1.76	0.66
1:B:65:ILE:HG22	1:B:69:MET:CE	2.23	0.66
1:B:695:LEU:HD12	1:B:825:MET:HE3	1.76	0.66
1:C:39:ALA:CB	1:C:673:GLU:HG2	2.25	0.66
1:C:367:ILE:CD1	1:C:492:LEU:HB3	2.26	0.66
1:B:727:PHE:HE1	1:B:786:ILE:HD11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:818:ARG:HG3	1:B:818:ARG:HH11	1.60	0.65
1:C:185:ARG:HH22	1:C:774:MET:HE3	1.61	0.65
1:A:445:ILE:HG21	1:A:940:LYS:HD2	1.78	0.65
1:A:782:LEU:O	1:A:785:ASP:HB2	1.97	0.65
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.77	0.65
1:A:886:LEU:HD21	1:C:17:ILE:HG22	1.77	0.65
1:C:9:PRO:HD2	1:C:10:ILE:HD13	1.78	0.65
1:B:326:PRO:HG3	1:B:610:PHE:CD1	2.32	0.65
1:A:911:GLY:HA2	1:A:914:LEU:HB2	1.77	0.65
1:A:979:SER:O	1:A:983:ILE:HG23	1.97	0.65
1:B:213:GLN:HE21	1:B:239:ARG:HD2	1.60	0.65
1:B:601:LYS:O	1:B:602:GLU:HG2	1.97	0.65
1:B:57:VAL:HG13	1:B:82:SER:OG	1.97	0.65
1:C:518:ARG:HA	1:C:518:ARG:HH21	1.62	0.65
1:A:584:GLN:N	1:A:622:GLN:HB3	2.11	0.64
1:B:103:ALA:O	1:B:107:VAL:HG23	1.97	0.64
1:C:848:ALA:HA	1:C:851:LEU:CD2	2.27	0.64
1:B:222:THR:CB	1:B:223:PRO:CD	2.74	0.64
1:A:221:GLY:CA	1:B:622:GLN:HE22	2.10	0.64
1:A:335:ILE:HG13	1:A:336:SER:N	2.12	0.64
1:A:989:LEU:HB3	1:A:993:THR:HG23	1.79	0.64
1:C:415:ASN:CG	1:C:434:SER:HB2	2.23	0.64
1:C:448:VAL:HG22	1:C:884:VAL:HG22	1.79	0.64
1:B:613:ASN:O	1:B:615:PHE:N	2.30	0.64
1:B:314:GLU:N	1:B:315:PRO:CD	2.61	0.64
1:B:879:ILE:O	1:B:883:VAL:HG23	1.96	0.64
1:B:905:VAL:CG1	1:B:906:PRO:HD3	2.27	0.64
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.26	0.64
1:A:330:THR:H	1:A:331:PRO:HD2	1.63	0.64
1:C:137:LEU:O	1:C:329:THR:HG22	1.98	0.64
1:B:850:LYS:C	1:B:852:PRO:HD3	2.23	0.64
1:C:1025:PHE:O	1:C:1029:VAL:HG23	1.97	0.64
1:A:632:LYS:O	1:A:637:ARG:HD3	1.98	0.64
1:B:904:VAL:HG13	1:B:907:LEU:HD12	1.80	0.64
1:A:154:ILE:O	1:A:158:VAL:HG23	1.97	0.64
1:B:527:TYR:HA	1:B:530:SER:HB2	1.80	0.63
1:B:699:ARG:HG2	1:B:700:ASN:H	1.63	0.63
1:A:317:PHE:HB3	1:A:321:LEU:HD21	1.79	0.63
1:C:1032:ARG:O	1:C:1035:ARG:HG2	1.97	0.63
1:A:11:PHE:CD1	1:B:890:ALA:HB1	2.32	0.63
1:A:712:MET:HA	1:A:832:ALA:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.79	0.63
1:B:754:TRP:CZ3	1:B:780:ARG:HA	2.33	0.63
1:B:918:PHE:CD1	1:B:919:ARG:HD3	2.30	0.63
1:C:144:ASN:ND2	1:C:148:THR:H	1.95	0.63
1:C:911:GLY:HA3	1:C:1013:THR:CB	2.27	0.63
1:A:1015:THR:C	1:A:1017:LEU:H	2.05	0.63
1:C:720:GLY:HA3	2:C:2002:RFP:H17C	1.81	0.63
1:C:925:VAL:O	1:C:927:PHE:N	2.32	0.63
1:A:667:ASN:C	1:A:667:ASN:HD22	2.06	0.63
1:B:1025:PHE:O	1:B:1029:VAL:HG12	1.98	0.63
1:C:435:MET:HA	1:C:438:ILE:HG22	1.81	0.63
1:C:646:ALA:HA	1:C:649:MET:HB2	1.81	0.63
1:C:897:ILE:N	1:C:898:PRO:HD2	2.13	0.63
1:A:218:GLN:O	1:A:219:LEU:HG	1.98	0.63
1:B:62:THR:O	1:B:66:GLU:HG3	1.99	0.63
1:A:254:ASN:ND2	1:A:258:SER:OG	2.31	0.62
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.99	0.62
1:B:231:ASN:C	1:B:231:ASN:HD22	2.06	0.62
1:B:605:ASN:HD22	1:B:605:ASN:H	1.47	0.62
1:C:265:VAL:O	1:C:266:ALA:HB2	1.99	0.62
1:C:34:GLN:HG3	1:C:333:VAL:CG1	2.29	0.62
1:C:1030:ARG:HH11	1:C:1030:ARG:HG2	1.65	0.62
1:C:1035:ARG:HE	1:C:1035:ARG:HA	1.64	0.62
1:C:23:GLY:HA3	1:C:377:LEU:O	1.99	0.62
1:C:688:ALA:O	1:C:689:GLY:O	2.16	0.62
1:A:686:ASP:HB3	1:A:823:PRO:HG2	1.81	0.62
1:C:26:ALA:O	1:C:30:LEU:HB2	1.99	0.62
1:B:136:PHE:HD1	1:B:136:PHE:H	1.47	0.62
1:C:953:MET:HE1	1:C:1030:ARG:NE	2.13	0.62
1:B:137:LEU:HD13	1:B:293:LEU:HG	1.81	0.62
1:B:888:LEU:C	1:B:890:ALA:H	2.06	0.62
1:C:204:ILE:CD1	1:C:773:VAL:HG21	2.30	0.62
1:C:712:MET:SD	1:C:843:LEU:HD22	2.40	0.62
1:C:901:VAL:O	1:C:904:VAL:HG23	1.98	0.62
1:B:249:ILE:HB	1:B:262:LEU:HB2	1.82	0.62
1:A:391:ASN:H	1:A:394:THR:HG22	1.64	0.62
1:A:418:ARG:HH21	1:A:970:MET:C	2.07	0.62
1:B:155:SER:OG	1:B:179:GLY:HA3	1.99	0.62
1:B:456:MET:HG3	1:B:467:TYR:CB	2.19	0.62
1:A:883:VAL:O	1:A:887:CYS:HB2	1.99	0.61
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:ILE:HG13	1:B:730:ASP:N	2.16	0.61
1:C:756:GLY:HA2	1:C:774:MET:HG3	1.81	0.61
1:A:83:ASP:HB3	1:A:815:ARG:HG3	1.82	0.61
1:A:713:LEU:HD22	1:A:714:THR:H	1.64	0.61
1:A:1013:THR:O	1:A:1017:LEU:HB3	1.99	0.61
1:B:921:LEU:HD22	1:B:1005:THR:HB	1.82	0.61
1:C:327:TYR:HB2	1:C:628:PHE:HB3	1.82	0.61
1:C:692:HIS:CE1	1:C:721:LEU:HD21	2.34	0.61
1:A:643:LYS:O	1:A:647:ILE:HG13	2.00	0.61
1:A:667:ASN:HD22	1:A:668:LEU:N	1.99	0.61
1:B:906:PRO:HA	1:B:909:VAL:HG22	1.83	0.61
1:B:251:LEU:HD12	1:B:262:LEU:HA	1.82	0.61
1:C:686:ASP:C	1:C:686:ASP:OD2	2.43	0.61
1:A:620:ARG:H	1:A:620:ARG:HD2	1.64	0.61
1:B:790:TYR:CD1	1:B:800:PRO:HA	2.36	0.61
1:B:925:VAL:HA	1:B:928:GLN:OE1	2.00	0.61
1:C:39:ALA:HB1	1:C:673:GLU:HG2	1.82	0.61
1:C:1004:GLY:O	1:C:1006:GLY:N	2.33	0.61
1:C:736:ALA:HB1	1:C:741:VAL:HG23	1.83	0.61
1:B:225:VAL:H	1:C:781:MET:CE	2.08	0.61
1:B:300:LEU:HD11	1:B:334:LYS:HE2	1.82	0.61
1:B:651:ALA:HB1	1:B:655:PHE:HE2	1.65	0.61
1:C:309:GLU:HG3	1:C:313:MET:CE	2.31	0.61
1:A:781:MET:HE2	1:C:225:VAL:H	1.65	0.61
1:C:379:THR:CG2	1:C:398:MET:HE1	2.31	0.61
1:C:888:LEU:C	1:C:890:ALA:H	2.09	0.61
1:A:317:PHE:HB3	1:A:321:LEU:HD23	1.82	0.60
1:B:185:ARG:NH2	1:B:774:MET:HE2	2.14	0.60
1:B:291:ILE:HG21	1:B:306:ILE:HD11	1.80	0.60
1:B:669:PRO:HB2	1:B:862:MET:HE2	1.81	0.60
1:B:736:ALA:HB2	1:B:804:PHE:CB	2.31	0.60
1:C:1:MET:HG3	1:C:3:ASN:H	1.66	0.60
1:C:423:GLU:HB3	1:C:426:PRO:HD2	1.82	0.60
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.83	0.60
1:C:144:ASN:ND2	1:C:148:THR:N	2.48	0.60
1:A:280:GLU:HB2	1:A:284:GLN:O	2.01	0.60
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.36	0.60
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.83	0.60
1:C:57:VAL:HG21	1:C:86:GLY:CA	2.29	0.60
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.83	0.60
1:A:108:GLN:HG2	1:A:129:VAL:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:GLY:HA3	1:B:1013:THR:CG2	2.31	0.60
1:C:99:ASP:OD2	1:C:102:ILE:HG12	2.02	0.60
1:C:176:GLN:HE22	1:C:620:ARG:HH12	1.49	0.60
1:C:477:ALA:C	1:C:479:ALA:H	2.10	0.60
1:B:591:LEU:O	1:B:595:THR:HG22	2.02	0.60
1:B:616:GLY:HA3	1:B:624:THR:CG2	2.32	0.60
1:A:6:ILE:CG2	1:A:490:PRO:HB2	2.31	0.60
1:B:741:VAL:HG21	1:B:791:VAL:HG23	1.83	0.60
1:A:1018:ALA:O	1:A:1022:VAL:HG22	2.01	0.59
1:B:736:ALA:HB2	1:B:804:PHE:HB3	1.83	0.59
1:B:911:GLY:HA2	1:B:914:LEU:HB3	1.84	0.59
1:C:350:LEU:C	1:C:352:PHE:H	2.10	0.59
1:A:443:VAL:HG22	1:A:486:LEU:HD11	1.84	0.59
1:B:919:ARG:CG	1:B:1005:THR:HG21	2.30	0.59
1:B:969:ARG:HH12	1:B:970:MET:HE3	1.67	0.59
1:A:57:VAL:HG13	1:A:88:VAL:CG2	2.32	0.59
1:C:9:PRO:HB3	1:C:491:ALA:HB1	1.84	0.59
1:C:365:THR:HG22	1:C:365:THR:O	2.02	0.59
1:B:921:LEU:CD2	1:B:1005:THR:HB	2.32	0.59
1:A:395:MET:HE2	1:A:395:MET:HA	1.83	0.59
1:B:213:GLN:HB2	1:B:239:ARG:HD2	1.84	0.59
1:C:326:PRO:HG3	1:C:610:PHE:CD1	2.38	0.59
1:C:394:THR:HG22	1:C:395:MET:HE3	1.85	0.59
1:C:835:LYS:HB3	1:C:839:GLU:OE2	2.01	0.59
1:A:600:THR:HG23	1:A:601:LYS:N	2.18	0.59
1:A:671:ILE:HB	1:A:674:LEU:HB3	1.84	0.59
1:B:144:ASN:HD21	1:B:148:THR:N	2.00	0.59
1:B:997:SER:C	1:B:999:ALA:H	2.10	0.59
1:C:592:ASN:O	1:C:593:GLU:HB2	2.01	0.59
1:A:713:LEU:HB2	1:A:832:ALA:HA	1.83	0.59
1:B:276:ASP:O	1:B:614:GLY:HA3	2.03	0.59
1:C:367:ILE:N	1:C:368:PRO:CD	2.66	0.59
1:C:547:ILE:HA	1:C:550:VAL:HG12	1.85	0.59
1:C:713:LEU:HD12	1:C:835:LYS:H	1.66	0.59
1:B:362:PHE:HA	1:B:365:THR:HG22	1.84	0.59
1:A:688:ALA:C	1:A:690:LEU:H	2.10	0.59
1:C:375:VAL:HG13	1:C:480:LEU:HB2	1.82	0.59
1:B:139:VAL:O	1:B:140:VAL:C	2.44	0.58
1:B:552:MET:SD	1:B:909:VAL:CG2	2.88	0.58
1:C:220:GLY:HA3	1:C:231:ASN:ND2	2.18	0.58
1:C:914:LEU:O	1:C:915:ALA:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:938:SER:O	1:C:941:ASN:ND2	2.36	0.58
1:A:441:ALA:O	1:A:445:ILE:HG23	2.02	0.58
1:A:442:LEU:C	1:A:444:GLY:H	2.12	0.58
1:B:104:GLN:HE22	1:B:108:GLN:NE2	2.01	0.58
1:B:523:SER:HA	1:B:526:HIS:HD2	1.67	0.58
1:C:340:VAL:HG12	1:C:340:VAL:O	2.04	0.58
1:C:401:ALA:O	1:C:405:LEU:HG	2.03	0.58
1:C:945:ILE:O	1:C:947:GLU:N	2.35	0.58
1:A:6:ILE:HD11	1:A:432:ARG:HG2	1.85	0.58
1:A:668:LEU:CD2	1:A:668:LEU:H	2.15	0.58
1:A:108:GLN:HE22	1:B:112:GLN:HB3	1.67	0.58
1:A:415:ASN:HD21	1:A:948:PHE:HZ	1.50	0.58
1:A:776:GLU:HB3	1:A:779:TYR:HD1	1.68	0.58
1:B:651:ALA:O	1:B:655:PHE:CD2	2.57	0.58
1:B:680:PHE:CD1	1:B:859:TRP:HZ3	2.20	0.58
1:C:746:ILE:HD13	1:C:791:VAL:HG11	1.86	0.58
1:A:578:LEU:CD2	1:A:587:THR:HG23	2.34	0.58
1:B:326:PRO:HG3	1:B:610:PHE:HD1	1.68	0.58
1:A:38:ILE:HD11	1:A:674:LEU:HG	1.85	0.58
1:A:210:GLN:HE22	1:A:250:LEU:H	1.51	0.58
1:A:360:GLN:HB2	1:A:513:PHE:CB	2.33	0.58
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.86	0.58
1:A:813:SER:HB3	1:A:816:LEU:CD2	2.33	0.58
1:C:378:GLY:O	1:C:382:VAL:HG23	2.04	0.58
1:C:497:LEU:HD12	1:C:498:LYS:HG3	1.85	0.58
1:A:400:LEU:HD22	1:A:1003:VAL:HG13	1.86	0.58
1:B:200:PRO:CD	1:B:749:THR:HG22	2.22	0.58
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.84	0.58
1:C:186:ILE:O	1:C:186:ILE:HG22	2.03	0.58
1:C:564:LEU:HD13	1:C:671:ILE:CD1	2.23	0.58
1:B:69:MET:HG2	1:B:92:LEU:HD11	1.86	0.58
1:B:346:GLU:O	1:B:350:LEU:HB2	2.04	0.58
1:B:1022:VAL:HA	1:B:1025:PHE:CD1	2.38	0.58
1:B:528:THR:OG1	1:B:969:ARG:HB2	2.04	0.58
1:B:911:GLY:N	1:B:1013:THR:HG21	2.19	0.58
1:C:188:MET:HE1	1:C:200:PRO:CA	2.27	0.58
1:C:713:LEU:HD23	1:C:831:ALA:CA	2.32	0.58
1:B:445:ILE:CG2	1:B:940:LYS:HG3	2.33	0.57
1:B:671:ILE:C	1:B:673:GLU:N	2.61	0.57
1:B:897:ILE:HD13	1:B:898:PRO:HD3	1.86	0.57
1:A:144:ASN:HB2	1:A:149:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ALA:O	1:A:709:HIS:N	2.36	0.57
1:A:740:GLY:CA	1:A:793:ALA:HB1	2.34	0.57
1:B:143:ILE:CG2	1:B:286:ALA:HB2	2.34	0.57
1:B:573:MET:HE3	1:B:628:PHE:CE2	2.39	0.57
1:C:485:ALA:O	1:C:490:PRO:HD3	2.04	0.57
1:C:695:LEU:HD22	1:C:825:MET:SD	2.44	0.57
1:B:166:ILE:HG21	1:B:291:ILE:HD12	1.86	0.57
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.84	0.57
1:B:53:ASP:HB2	1:B:56:THR:OG1	2.04	0.57
1:B:416:VAL:HG21	1:B:431:THR:HA	1.86	0.57
1:B:523:SER:HA	1:B:526:HIS:CD2	2.39	0.57
1:B:911:GLY:H	1:B:1013:THR:HG21	1.68	0.57
1:B:934:THR:HA	1:B:937:LEU:HD12	1.86	0.57
1:C:225:VAL:O	1:C:226:LYS:C	2.46	0.57
1:C:713:LEU:CD2	1:C:831:ALA:HA	2.31	0.57
1:B:104:GLN:HE22	1:B:108:GLN:HE21	1.50	0.57
1:C:406:VAL:O	1:C:408:ASP:N	2.37	0.57
1:C:1018:ALA:O	1:C:1022:VAL:HG23	2.04	0.57
1:B:158:VAL:HA	1:B:162:MET:CG	2.34	0.57
1:B:449:LEU:HD23	1:B:478:MET:CE	2.34	0.57
1:C:514:GLY:C	1:C:516:PHE:H	2.12	0.57
1:A:297:ALA:HB1	1:A:302:THR:HG21	1.87	0.57
1:C:143:ILE:HD11	1:C:281:PHE:HB3	1.85	0.57
1:C:946:VAL:HG12	1:C:946:VAL:O	2.04	0.57
1:A:225:VAL:HB	1:B:781:MET:HE3	1.87	0.57
1:A:832:ALA:O	1:A:833:PRO:C	2.48	0.57
1:A:775:SER:O	1:A:780:ARG:NH1	2.38	0.57
1:A:800:PRO:O	1:A:803:ALA:HB3	2.04	0.57
1:B:271:GLY:HA3	1:B:275:TYR:OH	2.05	0.57
1:C:952:LEU:O	1:C:953:MET:HG3	2.04	0.57
1:C:230:LEU:C	1:C:230:LEU:HD13	2.30	0.56
1:C:894:SER:O	1:C:898:PRO:HD3	2.04	0.56
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.87	0.56
1:B:24:GLY:H	1:B:27:ILE:HG23	1.69	0.56
1:C:10:ILE:HD13	1:C:10:ILE:H	1.69	0.56
1:A:872:GLN:O	1:A:876:LEU:HB2	2.06	0.56
1:B:282:ASN:C	1:B:284:GLN:H	2.12	0.56
1:B:332:PHE:CD1	1:B:569:GLN:HA	2.39	0.56
1:B:699:ARG:O	1:B:701:GLN:N	2.34	0.56
1:B:914:LEU:O	1:B:917:THR:HB	2.05	0.56
1:C:137:LEU:HD13	1:C:293:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ASN:ND2	1:C:149:MET:H	2.04	0.56
1:C:395:MET:O	1:C:398:MET:N	2.38	0.56
1:B:300:LEU:HD12	1:B:300:LEU:O	2.06	0.56
1:C:463:THR:HG22	1:C:464:GLY:H	1.71	0.56
1:A:746:ILE:HG12	1:A:804:PHE:CE1	2.41	0.56
1:A:991:ILE:HD11	1:A:1005:THR:N	2.21	0.56
1:B:10:ILE:CD1	1:C:893:GLU:O	2.53	0.56
1:B:391:ASN:O	1:B:395:MET:HG2	2.04	0.56
1:C:3:ASN:HD21	1:C:432:ARG:HG3	1.70	0.56
1:B:736:ALA:HB1	1:B:741:VAL:CG1	2.35	0.56
1:C:680:PHE:CZ	1:C:829:GLY:HA3	2.40	0.56
1:B:57:VAL:O	1:B:61:VAL:HG12	2.05	0.56
1:B:67:GLN:O	1:B:70:ASN:ND2	2.34	0.56
1:A:65:ILE:HD11	1:A:90:ILE:HD13	1.88	0.56
1:C:294:ALA:HB3	1:C:297:ALA:HB2	1.87	0.56
1:C:444:GLY:HA3	1:C:891:LEU:HD13	1.86	0.56
1:C:641:GLU:O	1:C:650:ARG:NH1	2.38	0.56
1:C:643:LYS:O	1:C:647:ILE:CG1	2.54	0.56
1:A:379:THR:HG21	1:A:477:ALA:CA	2.18	0.56
1:B:30:LEU:HD22	1:B:390:ILE:HG13	1.87	0.56
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.41	0.56
1:B:404:LEU:HD22	1:B:449:LEU:HD21	1.88	0.56
1:C:987:MET:SD	1:C:1008:MET:HE1	2.46	0.56
1:A:62:THR:O	1:A:66:GLU:HG2	2.05	0.56
1:A:246:PHE:O	1:A:249:ILE:HG13	2.05	0.56
1:A:740:GLY:HA3	1:A:793:ALA:HB1	1.88	0.56
1:C:134:SER:O	1:C:292:LYS:HE2	2.06	0.56
1:C:379:THR:OG1	1:C:477:ALA:HB2	2.06	0.56
1:A:584:GLN:H	1:A:622:GLN:HB3	1.71	0.55
1:B:59:ASP:HA	1:B:63:GLN:HG2	1.88	0.55
1:B:282:ASN:O	1:B:284:GLN:N	2.39	0.55
1:B:734:GLU:C	1:B:736:ALA:N	2.59	0.55
1:B:742:SER:HB3	1:B:745:ASP:OD2	2.05	0.55
1:B:1009:GLY:O	1:B:1012:VAL:HG22	2.06	0.55
1:C:199:THR:OG1	1:C:201:VAL:N	2.39	0.55
1:C:888:LEU:O	1:C:890:ALA:N	2.33	0.55
1:C:979:SER:O	1:C:983:ILE:HG13	2.07	0.55
1:C:228:GLN:HG3	1:C:229:GLN:O	2.06	0.55
1:C:379:THR:HG21	1:C:398:MET:CE	2.36	0.55
1:B:360:GLN:O	1:B:361:ASN:CB	2.53	0.55
1:C:166:ILE:HG21	1:C:291:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:PHE:C	1:C:615:PHE:CD2	2.85	0.55
1:A:253:VAL:HG13	1:A:253:VAL:O	2.04	0.55
1:A:552:MET:HB2	1:A:910:ILE:HG23	1.86	0.55
1:A:775:SER:HB2	1:A:789:TRP:CZ2	2.42	0.55
1:C:242:SER:OG	1:C:244:GLU:HB3	2.06	0.55
1:C:692:HIS:HE1	1:C:721:LEU:HD21	1.70	0.55
1:A:668:LEU:H	1:A:668:LEU:HD23	1.71	0.55
1:B:193:LEU:HG	1:B:265:VAL:HG22	1.88	0.55
1:B:370:ILE:O	1:B:370:ILE:CG2	2.55	0.55
1:B:448:VAL:O	1:B:452:VAL:HG23	2.05	0.55
1:B:708:LYS:C	1:B:710:PRO:HD3	2.31	0.55
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.22	0.55
1:C:1024:VAL:O	1:C:1028:VAL:HG23	2.06	0.55
1:A:184:MET:HE3	1:A:246:PHE:CD2	2.41	0.55
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.21	0.55
1:B:166:ILE:C	1:B:168:ARG:H	2.14	0.55
1:C:746:ILE:HD12	1:C:804:PHE:CZ	2.42	0.55
1:C:541:TYR:C	1:C:543:VAL:H	2.13	0.55
1:C:818:ARG:HA	1:C:824:SER:H	1.70	0.55
1:B:53:ASP:O	1:B:54:ALA:HB2	2.06	0.55
1:C:688:ALA:O	1:C:689:GLY:C	2.50	0.55
1:C:953:MET:SD	1:C:963:ALA:CB	2.92	0.55
1:B:219:LEU:HG	1:B:234:ILE:CD1	2.26	0.55
1:B:239:ARG:NH2	1:B:761:ASP:HB2	2.22	0.55
1:B:649:MET:O	1:B:653:ARG:HB2	2.07	0.55
1:B:790:TYR:HE1	1:B:800:PRO:HB3	1.71	0.55
1:B:986:VAL:O	1:B:990:VAL:HG23	2.07	0.55
1:C:65:ILE:HD13	1:C:111:LEU:CD2	2.37	0.55
1:C:908:GLY:CA	1:C:1014:ALA:HB2	2.34	0.55
1:A:278:ILE:HB	1:A:613:ASN:HB3	1.88	0.54
1:A:451:ALA:O	1:A:452:VAL:HG22	2.06	0.54
1:A:159:ALA:HB2	1:A:177:LEU:CD2	2.37	0.54
1:B:808:ARG:HH21	1:B:808:ARG:HB2	1.71	0.54
1:B:731:ILE:HG21	1:B:746:ILE:HG21	1.89	0.54
1:C:38:ILE:CG2	1:C:466:ILE:HD11	2.37	0.54
1:C:156:ASP:O	1:C:157:TYR:C	2.51	0.54
1:C:727:PHE:CZ	1:C:807:SER:CB	2.90	0.54
1:A:894:SER:OG	1:A:897:ILE:HB	2.07	0.54
1:B:1012:VAL:HG23	1:B:1013:THR:H	1.73	0.54
1:C:655:PHE:C	1:C:657:GLN:N	2.65	0.54
1:A:301:ASP:C	1:A:303:ALA:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:VAL:HG23	1:A:1023:PRO:HD3	1.89	0.54
1:A:1029:VAL:O	1:A:1030:ARG:HB2	2.07	0.54
1:B:605:ASN:H	1:B:605:ASN:ND2	2.05	0.54
1:C:1013:THR:O	1:C:1017:LEU:HB3	2.06	0.54
1:A:707:ALA:C	1:A:709:HIS:N	2.65	0.54
1:B:859:TRP:HB3	1:B:863:SER:HB3	1.90	0.54
1:A:659:LYS:HG2	1:A:660:ASP:N	2.23	0.54
1:B:404:LEU:HD21	1:B:937:LEU:HD23	1.89	0.54
1:B:544:LEU:O	1:B:548:ILE:HG12	2.07	0.54
1:C:895:TRP:CE3	1:C:895:TRP:HA	2.43	0.54
1:A:606:VAL:HA	1:A:631:LEU:HD23	1.90	0.54
1:B:185:ARG:CG	1:B:185:ARG:NH1	2.66	0.54
1:B:416:VAL:HG11	1:B:431:THR:HG22	1.90	0.54
1:B:452:VAL:O	1:B:453:PHE:CB	2.56	0.54
1:B:613:ASN:O	1:B:625:GLY:HA2	2.08	0.54
1:B:1022:VAL:HG23	1:B:1023:PRO:CD	2.37	0.54
1:C:131:LYS:HB2	1:C:295:THR:HG22	1.90	0.54
1:C:782:LEU:HB3	1:C:783:PRO:HD2	1.90	0.54
1:A:340:VAL:HG13	1:A:399:VAL:CG2	2.38	0.54
1:B:578:LEU:HB3	1:B:579:PRO:HD2	1.89	0.54
1:B:945:ILE:HG13	1:B:946:VAL:N	2.23	0.54
1:C:741:VAL:HG13	1:C:793:ALA:HB2	1.90	0.54
1:C:904:VAL:HA	1:C:907:LEU:HD23	1.90	0.54
1:A:563:PHE:O	1:A:564:LEU:HD23	2.08	0.54
1:A:685:ILE:HG22	1:A:687:GLN:NE2	2.23	0.54
1:A:923:ASN:C	1:A:923:ASN:ND2	2.61	0.54
1:B:414:GLU:CD	1:B:974:PRO:HG3	2.32	0.54
1:A:210:GLN:O	1:A:240:LEU:HD11	2.08	0.53
1:A:479:ALA:O	1:A:483:LEU:HD23	2.07	0.53
1:A:634:TRP:H	1:A:634:TRP:HD1	1.50	0.53
1:A:786:ILE:O	1:A:787:GLY:C	2.52	0.53
1:B:916:ALA:HA	1:B:919:ARG:HG2	1.90	0.53
1:C:158:VAL:HG12	1:C:177:LEU:HD21	1.91	0.53
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.90	0.53
1:B:905:VAL:HG13	1:B:906:PRO:CD	2.36	0.53
1:C:188:MET:HG3	1:C:774:MET:O	2.09	0.53
1:C:190:PRO:CD	1:C:779:TYR:CD1	2.91	0.53
1:C:605:ASN:ND2	1:C:637:ARG:HG2	2.24	0.53
1:A:31:PRO:HB3	1:A:296:GLY:HA2	1.90	0.53
1:A:172:VAL:O	1:A:172:VAL:HG23	2.08	0.53
1:A:783:PRO:HD3	1:C:219:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:VAL:HG12	1:C:932:LEU:HD22	1.89	0.53
1:C:801:PHE:O	1:C:803:ALA:N	2.40	0.53
1:B:158:VAL:HA	1:B:162:MET:HG2	1.89	0.53
1:B:841:MET:SD	1:B:866:GLU:OE2	2.66	0.53
1:C:792:ARG:CB	1:C:798:MET:HE1	2.36	0.53
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.90	0.53
1:C:361:ASN:HB3	1:C:364:ALA:HB3	1.89	0.53
1:C:590:VAL:O	1:C:594:VAL:HG23	2.09	0.53
1:A:420:MET:HE1	1:A:498:LYS:HA	1.89	0.53
1:A:709:HIS:N	1:A:710:PRO:HD3	2.24	0.53
1:B:178:PHE:CD1	1:B:612:VAL:HG11	2.43	0.53
1:B:220:GLY:HA2	1:C:781:MET:SD	2.49	0.53
1:B:314:GLU:HA	1:B:317:PHE:CE2	2.42	0.53
1:C:371:ALA:HB2	1:C:488:LEU:HD23	1.91	0.53
1:C:246:PHE:O	1:C:249:ILE:HG12	2.09	0.53
1:C:837:THR:O	1:C:841:MET:HB2	2.09	0.53
1:C:1026:PHE:CE1	1:C:1030:ARG:HD2	2.44	0.53
2:C:2002:RFP:H401	2:C:2002:RFP:C18	2.39	0.53
1:A:708:LYS:O	1:A:709:HIS:CD2	2.62	0.53
1:B:485:ALA:HA	1:B:489:THR:OG1	2.08	0.53
1:B:983:ILE:HD12	1:B:1012:VAL:HG13	1.89	0.53
1:B:985:GLY:O	1:B:988:PRO:HD2	2.09	0.53
1:C:49:TYR:HE1	1:C:60:THR:HG21	1.74	0.53
1:B:291:ILE:HG21	1:B:306:ILE:HD13	1.90	0.53
1:B:426:PRO:HB3	1:B:430:ALA:CB	2.39	0.53
1:B:600:THR:OG1	1:B:601:LYS:N	2.42	0.53
1:B:600:THR:C	1:B:602:GLU:H	2.17	0.53
1:B:732:ASP:O	1:B:734:GLU:N	2.42	0.53
1:B:924:ASP:HB3	1:B:926:TYR:H	1.75	0.53
1:C:317:PHE:CD1	1:C:321:LEU:HD12	2.44	0.53
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.10	0.52
1:C:204:ILE:HD13	1:C:773:VAL:HG21	1.90	0.52
1:C:442:LEU:O	1:C:445:ILE:HG13	2.09	0.52
1:A:159:ALA:HB2	1:A:177:LEU:HD22	1.92	0.52
1:A:688:ALA:O	1:A:690:LEU:N	2.42	0.52
1:C:2:PRO:HB2	1:C:6:ILE:HD11	1.91	0.52
1:C:176:GLN:HE22	1:C:620:ARG:NH1	2.08	0.52
1:A:105:VAL:CG2	1:B:105:VAL:HG13	2.39	0.52
1:A:352:PHE:HA	1:A:365:THR:HB	1.92	0.52
1:B:316:PHE:HD1	1:C:854:GLY:HA2	1.74	0.52
1:C:157:TYR:O	1:C:161:ASN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:VAL:HG11	1:C:406:VAL:HG21	1.91	0.52
1:C:351:VAL:HG22	1:C:981:ALA:O	2.09	0.52
1:C:767:ARG:HD3	1:C:769:LYS:HE3	1.91	0.52
1:A:139:VAL:HG13	1:A:139:VAL:O	2.09	0.52
1:A:172:VAL:HG12	1:A:291:ILE:HG21	1.91	0.52
1:A:575:MET:HA	1:A:626:ILE:HD13	1.91	0.52
1:C:326:PRO:O	1:C:327:TYR:C	2.52	0.52
1:C:966:ASP:O	1:C:970:MET:HG3	2.09	0.52
1:A:194:ASN:ND2	1:A:790:TYR:CD2	2.77	0.52
1:B:715:SER:O	1:B:716:VAL:C	2.53	0.52
1:C:192:GLU:HB3	1:C:265:VAL:HB	1.91	0.52
1:C:222:THR:CG2	1:C:223:PRO:CD	2.66	0.52
1:C:708:LYS:C	1:C:710:PRO:HD3	2.35	0.52
1:A:337:ILE:CD1	1:A:395:MET:HG3	2.39	0.52
1:A:560:PRO:HB2	1:A:922:THR:HG22	1.92	0.52
1:A:746:ILE:HG22	1:A:747:ASN:N	2.24	0.52
1:B:183:ALA:O	1:B:185:ARG:N	2.42	0.52
1:B:356:TYR:O	1:B:360:GLN:N	2.38	0.52
1:B:556:PHE:C	1:B:558:ARG:H	2.17	0.52
1:B:675:GLY:O	1:B:677:ALA:N	2.43	0.52
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.28	0.52
1:B:860:THR:O	1:B:861:GLY:C	2.52	0.52
1:C:308:ALA:O	1:C:312:LYS:HG3	2.10	0.52
1:C:873:ALA:C	1:C:875:SER:H	2.18	0.52
1:A:919:ARG:HG3	1:A:920:GLY:N	2.24	0.52
1:B:404:LEU:HD21	1:B:937:LEU:CD2	2.39	0.52
1:C:249:ILE:O	1:C:261:LEU:HA	2.10	0.52
1:C:415:ASN:HA	1:C:418:ARG:HH21	1.73	0.52
1:C:655:PHE:C	1:C:657:GLN:H	2.16	0.52
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.92	0.52
1:A:240:LEU:HD12	1:A:240:LEU:N	2.25	0.52
1:A:299:ALA:O	1:A:303:ALA:HB2	2.10	0.52
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.44	0.52
1:C:592:ASN:HA	1:C:595:THR:OG1	2.10	0.52
1:B:699:ARG:HH11	1:B:699:ARG:CB	2.19	0.52
1:B:706:ALA:C	1:B:708:LYS:N	2.66	0.52
1:C:531:VAL:O	1:C:533:GLY:N	2.42	0.52
1:C:785:ASP:C	1:C:787:GLY:H	2.18	0.52
1:A:890:ALA:HB1	1:C:11:PHE:CD1	2.45	0.52
1:B:78:MET:HA	1:B:91:THR:O	2.10	0.52
1:C:463:THR:HA	1:C:466:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HG22	1:A:118:LEU:HD11	1.92	0.51
1:A:525:HIS:HA	1:A:528:THR:HG22	1.91	0.51
1:A:600:THR:O	1:A:603:LYS:HD3	2.09	0.51
1:B:973:ARG:HB3	1:B:974:PRO:HD3	1.93	0.51
1:C:400:LEU:HD11	1:C:930:GLY:HA2	1.92	0.51
1:C:482:VAL:O	1:C:486:LEU:HG	2.10	0.51
1:C:760:ASN:O	1:C:771:VAL:HG23	2.09	0.51
1:A:30:LEU:HD21	1:A:384:ALA:HB2	1.90	0.51
1:A:909:VAL:O	1:A:912:ALA:HB3	2.10	0.51
1:A:911:GLY:CA	1:A:914:LEU:HB2	2.41	0.51
1:A:1010:GLY:O	1:A:1014:ALA:HB2	2.11	0.51
1:B:189:ASN:HD22	1:B:190:PRO:HD2	1.76	0.51
1:B:462:SER:OG	1:B:865:GLN:HG2	2.10	0.51
1:B:919:ARG:HB2	1:B:921:LEU:HD13	1.91	0.51
1:C:329:THR:C	1:C:331:PRO:HD2	2.35	0.51
1:C:527:TYR:OH	1:C:968:VAL:HG12	2.09	0.51
1:C:574:THR:HG23	1:C:665:ALA:HB2	1.92	0.51
1:A:158:VAL:HA	1:A:162:MET:HG2	1.92	0.51
1:B:525:HIS:O	1:B:528:THR:HG22	2.09	0.51
1:C:76:MET:HE2	1:C:94:PHE:O	2.10	0.51
1:C:193:LEU:HB3	1:C:198:LEU:O	2.10	0.51
1:C:368:PRO:HD2	1:C:369:THR:H	1.75	0.51
1:C:420:MET:SD	1:C:498:LYS:HD3	2.51	0.51
1:C:983:ILE:CG2	1:C:1008:MET:HG3	2.38	0.51
1:A:862:MET:HA	1:A:865:GLN:HB3	1.93	0.51
1:C:361:ASN:HD22	1:C:362:PHE:N	2.08	0.51
1:A:38:ILE:CD1	1:A:674:LEU:HG	2.40	0.51
1:B:49:TYR:O	1:B:50:PRO:C	2.54	0.51
1:B:146:ASP:O	1:B:148:THR:N	2.44	0.51
1:C:400:LEU:CD1	1:C:930:GLY:HA2	2.41	0.51
1:C:415:ASN:HA	1:C:418:ARG:NH2	2.25	0.51
1:C:564:LEU:HD23	1:C:565:PRO:HD2	1.93	0.51
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.92	0.51
1:A:281:PHE:O	1:A:282:ASN:C	2.54	0.51
1:A:649:MET:HB3	1:A:653:ARG:HH22	1.75	0.51
1:B:166:ILE:HG21	1:B:291:ILE:CD1	2.41	0.51
1:A:298:ASN:HB2	1:A:301:ASP:H	1.76	0.51
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.93	0.51
1:B:566:ASP:C	1:B:567:GLU:HG2	2.35	0.51
1:C:946:VAL:HG13	1:C:1026:PHE:CD1	2.46	0.51
1:C:1016:VAL:O	1:C:1018:ALA:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:OD1	1:A:330:THR:HB	2.11	0.51
1:A:552:MET:HE1	1:A:906:PRO:CA	2.41	0.51
1:C:143:ILE:HD11	1:C:281:PHE:CB	2.40	0.51
1:C:819:TYR:N	1:C:824:SER:HB3	2.26	0.51
1:A:282:ASN:ND2	1:A:609:VAL:H	2.09	0.51
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.46	0.51
1:A:959:GLY:HA3	1:A:962:GLU:HB3	1.92	0.51
1:B:10:ILE:HD12	1:C:893:GLU:HG3	1.92	0.51
1:B:651:ALA:HB1	1:B:655:PHE:CE2	2.45	0.51
1:B:768:VAL:HG23	1:C:63:GLN:NE2	2.25	0.51
1:C:520:PHE:O	1:C:524:THR:HG23	2.10	0.51
1:C:577:GLN:CD	1:C:578:LEU:H	2.18	0.51
1:C:712:MET:O	1:C:713:LEU:C	2.54	0.51
1:C:832:ALA:HB3	1:C:833:PRO:CD	2.33	0.51
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.93	0.51
1:B:250:LEU:HD12	1:B:259:ARG:NH2	2.21	0.51
1:B:680:PHE:CE1	1:B:844:MET:HE2	2.45	0.51
1:C:131:LYS:O	1:C:295:THR:HG22	2.11	0.51
1:C:144:ASN:HD21	1:C:148:THR:H	1.57	0.51
1:A:400:LEU:HD11	1:A:930:GLY:CA	2.28	0.50
1:A:454:VAL:O	1:A:456:MET:N	2.44	0.50
1:A:813:SER:HB3	1:A:816:LEU:HD21	1.93	0.50
1:B:818:ARG:HG3	1:B:818:ARG:NH1	2.25	0.50
1:B:1028:VAL:O	1:B:1032:ARG:HB2	2.11	0.50
1:C:142:VAL:C	1:C:143:ILE:HD12	2.36	0.50
1:C:176:GLN:NE2	1:C:620:ARG:NH1	2.58	0.50
1:C:184:MET:HG2	1:C:246:PHE:CE1	2.46	0.50
1:C:474:ILE:O	1:C:478:MET:HB2	2.11	0.50
1:C:624:THR:HB	2:C:2002:RFP:H381	1.92	0.50
1:A:102:ILE:O	1:A:106:GLN:HG3	2.11	0.50
1:A:251:LEU:CD1	1:A:265:VAL:HG21	2.41	0.50
1:A:406:VAL:C	1:A:408:ASP:H	2.19	0.50
1:A:418:ARG:NH2	1:A:970:MET:O	2.44	0.50
1:A:454:VAL:C	1:A:456:MET:H	2.19	0.50
1:A:587:THR:OG1	1:A:622:GLN:O	2.26	0.50
1:A:987:MET:N	1:A:988:PRO:CD	2.74	0.50
1:B:213:GLN:HG2	1:C:56:THR:HG23	1.94	0.50
1:B:671:ILE:C	1:B:673:GLU:H	2.20	0.50
1:B:700:ASN:C	1:B:702:LEU:H	2.19	0.50
1:C:713:LEU:O	1:C:713:LEU:CD2	2.59	0.50
1:A:104:GLN:OE1	1:A:131:LYS:HE3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HE3	1:A:254:ASN:HB3	1.93	0.50
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.92	0.50
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.46	0.50
1:C:140:VAL:O	1:C:288:GLY:HA3	2.10	0.50
1:C:193:LEU:HD23	1:C:265:VAL:HG21	1.93	0.50
1:C:204:ILE:HD11	1:C:773:VAL:HG21	1.92	0.50
1:C:459:PHE:O	1:C:464:GLY:HA3	2.11	0.50
1:C:643:LYS:HE2	1:C:645:GLU:HB3	1.92	0.50
1:C:732:ASP:N	1:C:804:PHE:O	2.36	0.50
1:A:235:ILE:CD1	1:B:53:ASP:HB3	2.42	0.50
1:A:574:THR:HG21	1:A:594:VAL:CG1	2.39	0.50
1:C:391:ASN:H	1:C:394:THR:HB	1.77	0.50
1:C:1007:VAL:O	1:C:1011:MET:HB2	2.11	0.50
1:A:1019:ILE:HG12	1:A:1020:PHE:CD1	2.46	0.50
1:A:552:MET:HE2	1:A:909:VAL:HB	1.94	0.50
1:B:198:LEU:HD23	1:B:792:ARG:HH22	1.76	0.50
1:C:204:ILE:HG22	1:C:208:LYS:HD2	1.92	0.50
1:C:941:ASN:HD22	1:C:942:ALA:N	2.10	0.50
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.94	0.50
1:A:481:SER:O	1:A:484:VAL:HG22	2.11	0.50
1:A:575:MET:HE1	1:A:577:GLN:HE21	1.77	0.50
1:A:713:LEU:HB2	1:A:832:ALA:CA	2.42	0.50
1:B:376:LEU:HD11	1:B:402:ILE:HD13	1.94	0.50
1:B:560:PRO:HB3	1:B:839:GLU:OE1	2.12	0.50
1:C:352:PHE:HA	1:C:369:THR:HG21	1.92	0.50
1:A:6:ILE:HG22	1:A:490:PRO:HB2	1.93	0.50
1:B:143:ILE:HG23	1:B:286:ALA:HB2	1.93	0.50
1:B:987:MET:HB3	1:B:988:PRO:CD	2.37	0.50
1:A:235:ILE:HD13	1:B:53:ASP:HB3	1.93	0.50
1:A:780:ARG:HG2	1:A:780:ARG:NH1	2.26	0.50
1:C:342:LYS:C	1:C:344:LEU:H	2.18	0.50
1:C:786:ILE:HD12	1:C:786:ILE:H	1.77	0.50
1:A:108:GLN:NE2	1:B:112:GLN:CB	2.70	0.49
1:A:897:ILE:N	1:A:898:PRO:HD2	2.27	0.49
1:B:616:GLY:HA3	1:B:624:THR:HG21	1.93	0.49
1:B:1013:THR:HA	1:B:1017:LEU:HD13	1.93	0.49
1:C:476:SER:O	1:C:477:ALA:CB	2.59	0.49
1:C:949:ALA:HB1	1:C:1026:PHE:CZ	2.47	0.49
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.92	0.49
1:C:158:VAL:HG13	1:C:289:LEU:HD21	1.93	0.49
1:C:199:THR:OG1	1:C:201:VAL:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:THR:N	1:C:490:PRO:HD2	2.27	0.49
1:A:442:LEU:O	1:A:445:ILE:HG13	2.11	0.49
1:B:36:PRO:O	1:B:37:THR:C	2.53	0.49
1:C:190:PRO:HG3	1:C:789:TRP:CH2	2.46	0.49
1:C:380:PHE:HE1	1:C:398:MET:SD	2.32	0.49
1:C:757:SER:O	1:C:772:TYR:HA	2.12	0.49
1:A:585:GLU:OE2	1:C:227:GLY:HA2	2.12	0.49
1:A:590:VAL:O	1:A:594:VAL:HG23	2.13	0.49
1:B:55:LYS:O	1:B:57:VAL:N	2.37	0.49
1:B:138:MET:HG2	1:B:139:VAL:N	2.27	0.49
1:B:669:PRO:HG3	1:B:678:THR:HA	1.94	0.49
1:C:115:MET:HA	1:C:118:LEU:HD22	1.95	0.49
1:C:945:ILE:HG13	1:C:971:ARG:HG3	1.93	0.49
1:A:171:GLY:HA3	1:A:302:THR:HG21	1.95	0.49
1:A:228:GLN:HG2	1:B:781:MET:HG3	1.94	0.49
1:A:240:LEU:N	1:A:240:LEU:CD1	2.76	0.49
1:B:435:MET:HA	1:B:435:MET:CE	2.36	0.49
1:B:493:CYS:HA	1:B:497:LEU:HB2	1.94	0.49
1:C:314:GLU:HB2	1:C:315:PRO:HD3	1.94	0.49
1:C:349:ILE:O	1:C:352:PHE:HB3	2.13	0.49
1:C:382:VAL:HG11	1:C:476:SER:HB2	1.94	0.49
1:A:53:ASP:HA	1:A:84:SER:HA	1.93	0.49
1:A:447:MET:HB3	1:A:887:CYS:HG	1.73	0.49
1:A:578:LEU:HD21	1:A:587:THR:HG23	1.95	0.49
1:A:713:LEU:HD13	1:A:714:THR:N	2.27	0.49
1:B:450:SER:O	1:B:452:VAL:O	2.31	0.49
1:C:332:PHE:CD2	1:C:569:GLN:HA	2.47	0.49
1:C:437:GLN:O	1:C:438:ILE:HB	2.13	0.49
1:C:894:SER:C	1:C:896:SER:H	2.20	0.49
1:A:70:ASN:HB3	1:C:167:SER:HB3	1.95	0.49
1:A:634:TRP:CD1	1:A:634:TRP:N	2.66	0.49
1:B:454:VAL:O	1:B:455:PRO:C	2.54	0.49
1:C:721:LEU:HD13	1:C:825:MET:HE2	1.95	0.49
1:C:985:GLY:O	1:C:988:PRO:HD2	2.12	0.49
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.94	0.49
1:B:555:LEU:HA	1:B:558:ARG:HE	1.77	0.49
1:C:150:THR:O	1:C:154:ILE:HG13	2.12	0.49
1:C:586:ARG:O	1:C:590:VAL:HG23	2.13	0.49
1:C:685:ILE:O	1:C:685:ILE:CG1	2.61	0.49
1:C:752:ALA:O	1:C:774:MET:HA	2.13	0.49
1:A:171:GLY:O	1:A:172:VAL:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:ARG:HD2	1:A:780:ARG:O	2.13	0.49
1:A:813:SER:CB	1:A:816:LEU:HD23	2.42	0.49
1:A:899:PHE:HA	1:A:902:MET:HG3	1.94	0.49
1:B:139:VAL:O	1:B:139:VAL:CG1	2.47	0.49
1:C:345:VAL:O	1:C:348:ILE:N	2.40	0.49
1:C:355:MET:HG2	1:C:368:PRO:HG2	1.94	0.49
1:C:564:LEU:CD1	1:C:671:ILE:HD12	2.27	0.49
1:C:847:LEU:HD23	1:C:847:LEU:H	1.78	0.49
1:C:1013:THR:HG23	1:C:1014:ALA:N	2.26	0.49
1:A:843:LEU:O	1:A:843:LEU:HD22	2.13	0.49
1:B:605:ASN:ND2	1:B:605:ASN:N	2.60	0.49
1:C:815:ARG:NH1	1:C:815:ARG:CG	2.62	0.49
1:B:382:VAL:HG11	1:B:476:SER:OG	2.13	0.48
1:B:922:THR:OG1	1:B:923:ASN:N	2.45	0.48
1:C:40:PRO:HB2	1:C:94:PHE:O	2.12	0.48
1:C:655:PHE:O	1:C:657:GLN:N	2.46	0.48
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.93	0.48
1:B:184:MET:H	1:B:762:PHE:HE2	1.59	0.48
1:B:339:GLU:HG3	1:B:996:GLY:H	1.77	0.48
1:C:53:ASP:O	1:C:54:ALA:HB2	2.13	0.48
1:C:577:GLN:HG2	2:C:2002:RFP:C39	2.44	0.48
1:A:742:SER:O	1:A:743:ILE:C	2.54	0.48
1:A:1015:THR:C	1:A:1017:LEU:N	2.71	0.48
1:B:780:ARG:O	1:B:781:MET:HB2	2.13	0.48
1:C:344:LEU:HD23	1:C:399:VAL:HG22	1.94	0.48
1:C:736:ALA:C	1:C:738:ALA:H	2.22	0.48
1:A:239:ARG:HD3	1:A:762:PHE:HA	1.95	0.48
1:A:713:LEU:HD13	1:A:714:THR:H	1.78	0.48
1:C:399:VAL:O	1:C:402:ILE:HB	2.13	0.48
1:C:404:LEU:HD23	1:C:449:LEU:HD13	1.96	0.48
1:A:1015:THR:O	1:A:1017:LEU:N	2.47	0.48
1:B:776:GLU:OE1	1:B:778:LYS:HE2	2.13	0.48
1:C:419:VAL:HG23	1:C:430:ALA:HB1	1.94	0.48
1:C:841:MET:O	1:C:845:GLU:HG3	2.13	0.48
1:A:225:VAL:O	1:A:226:LYS:C	2.56	0.48
1:B:449:LEU:HD23	1:B:478:MET:HE2	1.96	0.48
1:B:531:VAL:O	1:B:535:LEU:HD23	2.13	0.48
1:B:723:ASP:HA	1:B:814:PRO:HD3	1.95	0.48
1:B:940:LYS:NZ	1:B:978:THR:HG22	2.29	0.48
1:C:907:LEU:HD12	1:C:1017:LEU:HG	1.95	0.48
1:A:188:MET:SD	1:A:200:PRO:HB3	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASP:OD2	1:A:301:ASP:N	2.46	0.48
1:A:340:VAL:HG13	1:A:399:VAL:HG23	1.96	0.48
1:B:947:GLU:O	1:B:947:GLU:HG3	2.14	0.48
1:C:672:VAL:HG13	1:C:676:THR:H	1.78	0.48
1:C:801:PHE:CD1	1:C:804:PHE:HE1	2.32	0.48
1:A:328:ASP:CG	1:A:330:THR:HB	2.39	0.48
1:B:197:GLN:HB3	1:B:798:MET:HE3	1.94	0.48
1:B:348:ILE:HG23	1:B:372:VAL:HG21	1.96	0.48
1:B:888:LEU:O	1:B:890:ALA:N	2.47	0.48
1:C:184:MET:HG2	1:C:246:PHE:CD1	2.49	0.48
1:C:624:THR:CB	2:C:2002:RFP:H381	2.44	0.48
1:A:21:LEU:O	1:A:25:LEU:HB2	2.14	0.48
1:A:142:VAL:CG1	1:A:321:LEU:HD12	2.43	0.48
1:A:605:ASN:OD1	1:A:637:ARG:HG2	2.14	0.48
1:A:692:HIS:CE1	1:A:813:SER:HB2	2.49	0.48
1:C:158:VAL:CG1	1:C:177:LEU:HD21	2.43	0.48
1:C:968:VAL:HG11	1:C:1023:PRO:CG	2.38	0.48
1:A:108:GLN:HB3	1:B:112:GLN:HE22	1.79	0.48
1:A:356:TYR:C	1:A:358:PHE:H	2.22	0.48
1:B:1017:LEU:HD12	1:B:1017:LEU:H	1.79	0.48
1:C:192:GLU:HG2	1:C:264:ASP:O	2.13	0.48
1:C:265:VAL:O	1:C:265:VAL:CG2	2.62	0.48
1:C:402:ILE:O	1:C:406:VAL:HG23	2.13	0.48
1:C:644:VAL:CG1	1:C:667:ASN:HB2	2.43	0.48
1:C:216:ALA:HB3	1:C:234:ILE:O	2.14	0.47
1:C:409:ALA:O	1:C:413:VAL:HG22	2.14	0.47
1:C:968:VAL:CG1	1:C:1023:PRO:HG3	2.36	0.47
1:C:997:SER:HA	1:C:1000:GLN:OE1	2.14	0.47
1:A:108:GLN:HB3	1:B:112:GLN:NE2	2.29	0.47
1:A:674:LEU:HD22	1:A:675:GLY:N	2.15	0.47
1:B:58:GLN:NE2	1:B:818:ARG:NH1	2.62	0.47
1:B:136:PHE:CD1	1:B:136:PHE:N	2.78	0.47
1:B:676:THR:HG22	1:B:676:THR:O	2.15	0.47
1:B:680:PHE:HE1	1:B:844:MET:HE2	1.78	0.47
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.79	0.47
1:C:888:LEU:C	1:C:890:ALA:N	2.72	0.47
1:C:895:TRP:HA	1:C:895:TRP:HE3	1.77	0.47
1:B:19:ILE:HG22	1:B:378:GLY:HA3	1.97	0.47
1:C:577:GLN:CD	1:C:578:LEU:N	2.72	0.47
1:A:30:LEU:CD2	1:A:384:ALA:HB2	2.45	0.47
1:A:668:LEU:N	1:A:668:LEU:HD23	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:THR:HB	1:B:223:PRO:HD2	1.90	0.47
1:B:351:VAL:O	1:B:352:PHE:C	2.57	0.47
1:B:372:VAL:HB	1:B:402:ILE:CD1	2.41	0.47
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.95	0.47
1:C:210:GLN:NE2	1:C:250:LEU:H	2.11	0.47
1:C:569:GLN:C	1:C:634:TRP:HZ2	2.23	0.47
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.49	0.47
1:A:275:TYR:CB	1:C:223:PRO:CD	2.86	0.47
1:B:75:LEU:HD12	1:B:75:LEU:HA	1.75	0.47
1:B:156:ASP:OD2	1:B:182:TYR:HB2	2.15	0.47
1:B:568:ASP:HA	1:B:644:VAL:HG21	1.96	0.47
1:C:195:LYS:HE3	1:C:196:PHE:CE1	2.50	0.47
1:C:303:ALA:O	1:C:307:ARG:HG2	2.14	0.47
1:C:331:PRO:O	1:C:332:PHE:C	2.57	0.47
1:C:467:TYR:CE2	1:C:925:VAL:HG12	2.50	0.47
1:A:6:ILE:HD11	1:A:432:ARG:CG	2.44	0.47
1:B:240:LEU:HB2	1:B:246:PHE:CE2	2.50	0.47
1:B:696:THR:HA	1:B:699:ARG:NH1	2.30	0.47
1:B:713:LEU:HD23	1:B:716:VAL:HG21	1.96	0.47
1:B:852:PRO:HB2	1:B:853:THR:H	1.54	0.47
1:B:915:ALA:O	1:B:917:THR:N	2.44	0.47
1:C:692:HIS:NE2	1:C:813:SER:HB2	2.30	0.47
1:A:192:GLU:O	1:A:265:VAL:HG12	2.15	0.47
1:A:596:HIS:O	1:A:597:TYR:C	2.58	0.47
1:A:843:LEU:HD22	1:A:847:LEU:HG	1.96	0.47
1:B:23:GLY:HA2	1:B:26:ALA:HB3	1.97	0.47
1:B:99:ASP:C	1:B:99:ASP:OD2	2.57	0.47
1:B:219:LEU:CG	1:B:234:ILE:HD11	2.30	0.47
1:B:256:ASP:OD1	1:B:256:ASP:N	2.44	0.47
1:B:768:VAL:HG23	1:C:63:GLN:CD	2.39	0.47
1:B:858:ASP:OD1	1:B:867:ARG:NH2	2.48	0.47
1:C:328:ASP:OD1	1:C:328:ASP:C	2.58	0.47
1:C:465:ALA:O	1:C:469:GLN:HG2	2.14	0.47
1:C:785:ASP:C	1:C:787:GLY:N	2.72	0.47
1:A:324:VAL:HG12	1:A:325:TYR:H	1.80	0.47
1:A:644:VAL:C	1:A:646:ALA:H	2.21	0.47
1:B:420:MET:HE2	1:B:426:PRO:HD3	1.97	0.47
1:B:528:THR:O	1:B:531:VAL:HG12	2.15	0.47
1:B:782:LEU:O	1:B:784:ASP:N	2.47	0.47
1:B:873:ALA:HB2	1:B:928:GLN:HE21	1.80	0.47
1:C:83:ASP:HB2	1:C:87:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:VAL:O	1:A:544:LEU:HB3	2.14	0.47
1:A:747:ASN:HD21	1:C:237:GLN:NE2	2.13	0.47
1:A:813:SER:HB3	1:A:816:LEU:HD23	1.96	0.47
1:A:953:MET:HE3	1:A:963:ALA:HB3	1.97	0.47
1:B:848:ALA:C	1:B:850:LYS:H	2.23	0.47
1:C:672:VAL:HG13	1:C:675:GLY:H	1.79	0.47
1:C:706:ALA:HB3	1:C:716:VAL:HG21	1.97	0.47
1:A:73:ASP:H	1:A:106:GLN:NE2	2.09	0.47
1:A:752:ALA:O	1:A:756:GLY:HA2	2.15	0.47
1:B:582:ALA:HB3	1:B:623:ASN:HB3	1.97	0.47
1:B:764:ASP:O	1:B:766:GLY:N	2.48	0.47
1:C:463:THR:O	1:C:465:ALA:N	2.41	0.47
1:C:748:THR:O	1:C:752:ALA:HB2	2.15	0.47
1:C:764:ASP:OD1	1:C:765:ARG:HG3	2.14	0.47
1:C:992:SER:HB3	1:C:997:SER:HB2	1.97	0.47
1:A:682:PHE:HD1	1:A:859:TRP:CH2	2.33	0.46
1:A:729:ILE:HD11	1:A:786:ILE:HD11	1.97	0.46
1:B:55:LYS:C	1:B:57:VAL:H	2.20	0.46
1:B:367:ILE:CG2	1:B:489:THR:HG23	2.45	0.46
1:C:30:LEU:HD11	1:C:380:PHE:O	2.15	0.46
1:C:230:LEU:HD13	1:C:230:LEU:O	2.15	0.46
1:C:915:ALA:HB1	1:C:1005:THR:HG22	1.96	0.46
1:B:143:ILE:HD12	1:B:322:LYS:HB3	1.97	0.46
1:B:193:LEU:HG	1:B:265:VAL:CG2	2.45	0.46
1:B:519:MET:HA	1:B:519:MET:HE2	1.97	0.46
1:B:762:PHE:HD2	1:B:771:VAL:HG22	1.79	0.46
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.51	0.46
1:A:231:ASN:OD1	1:B:622:GLN:NE2	2.49	0.46
1:A:934:THR:C	1:A:936:GLY:N	2.72	0.46
1:B:580:ALA:O	1:B:581:GLY:C	2.58	0.46
1:B:704:ALA:O	1:B:705:GLU:HB2	2.14	0.46
1:B:987:MET:HA	1:B:987:MET:HE3	1.97	0.46
1:C:911:GLY:HA3	1:C:1013:THR:HB	1.97	0.46
1:C:958:LYS:HD2	1:C:958:LYS:N	2.31	0.46
1:A:153:ASP:HA	1:A:182:TYR:OH	2.16	0.46
1:A:598:TYR:O	1:A:602:GLU:HB2	2.15	0.46
1:B:198:LEU:HD13	1:B:251:LEU:HD22	1.97	0.46
1:B:235:ILE:HD12	1:B:235:ILE:N	2.30	0.46
1:B:561:SER:O	1:B:838:GLY:HA3	2.16	0.46
1:C:189:ASN:C	1:C:189:ASN:HD22	2.23	0.46
1:C:813:SER:HB3	1:C:816:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:THR:HG23	1:A:601:LYS:H	1.78	0.46
1:A:740:GLY:O	1:A:794:ALA:N	2.41	0.46
1:B:137:LEU:HG	1:B:137:LEU:O	2.14	0.46
1:B:940:LYS:HZ1	1:B:978:THR:HG22	1.81	0.46
1:C:174:ASP:HB3	1:C:292:LYS:HB2	1.96	0.46
1:C:222:THR:O	1:C:223:PRO:C	2.58	0.46
1:C:897:ILE:N	1:C:898:PRO:CD	2.79	0.46
1:A:66:GLU:C	1:A:68:ASN:N	2.74	0.46
1:A:255:GLN:O	1:A:256:ASP:HB3	2.15	0.46
1:A:726:GLN:HB2	1:C:235:ILE:HD13	1.98	0.46
1:B:398:MET:O	1:B:402:ILE:HB	2.15	0.46
1:B:545:TYR:C	1:B:547:ILE:H	2.24	0.46
1:B:648:THR:HG23	1:B:665:ALA:O	2.15	0.46
1:B:892:TYR:HB2	1:B:897:ILE:CD1	2.41	0.46
1:B:964:THR:O	1:B:968:VAL:HG23	2.15	0.46
1:C:38:ILE:HG21	1:C:466:ILE:CD1	2.42	0.46
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.98	0.46
1:A:99:ASP:OD1	1:A:101:ASP:N	2.46	0.46
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.97	0.46
1:B:61:VAL:HG13	1:B:88:VAL:HG21	1.98	0.46
1:B:316:PHE:CD1	1:C:854:GLY:HA2	2.51	0.46
1:C:758:TYR:CE1	1:C:770:LYS:HD3	2.51	0.46
1:A:253:VAL:O	1:A:253:VAL:CG1	2.64	0.46
1:A:324:VAL:HG12	1:A:325:TYR:N	2.30	0.46
1:A:584:GLN:H	1:A:622:GLN:HE21	1.62	0.46
1:A:733:GLN:O	1:A:734:GLU:C	2.59	0.46
1:B:345:VAL:HA	1:B:348:ILE:HD12	1.97	0.46
1:B:369:THR:C	1:B:371:ALA:H	2.24	0.46
1:B:613:ASN:C	1:B:615:PHE:H	2.23	0.46
1:B:927:PHE:CE2	1:B:931:LEU:HD11	2.51	0.46
1:B:997:SER:C	1:B:999:ALA:N	2.73	0.46
1:C:160:ALA:HB1	1:C:767:ARG:HD2	1.98	0.46
1:C:213:GLN:NE2	1:C:238:THR:HA	2.31	0.46
1:C:263:ARG:HD3	1:C:268:ILE:HD12	1.98	0.46
1:A:180:SER:HB3	1:A:273:GLU:H	1.81	0.46
1:A:222:THR:O	1:A:223:PRO:C	2.59	0.46
1:A:330:THR:N	1:A:331:PRO:HD2	2.31	0.46
1:A:655:PHE:C	1:A:657:GLN:H	2.22	0.46
1:B:111:LEU:O	1:B:113:LEU:N	2.49	0.46
1:A:66:GLU:C	1:A:68:ASN:H	2.24	0.46
1:A:540:ARG:HD2	1:A:541:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:O	1:C:264:ASP:HB2	2.16	0.46
1:C:367:ILE:H	1:C:368:PRO:HD3	1.81	0.46
1:C:415:ASN:O	1:C:419:VAL:HG22	2.16	0.46
1:C:662:MET:H	1:C:662:MET:CE	2.24	0.46
1:C:780:ARG:O	1:C:780:ARG:HG3	2.16	0.46
1:A:533:GLY:C	1:A:535:LEU:H	2.24	0.45
1:A:600:THR:C	1:A:602:GLU:H	2.23	0.45
1:A:894:SER:CB	1:A:897:ILE:HD13	2.45	0.45
1:B:343:THR:HA	1:B:346:GLU:HG2	1.98	0.45
1:C:183:ALA:O	1:C:185:ARG:HG2	2.16	0.45
1:C:786:ILE:HD12	1:C:786:ILE:N	2.31	0.45
1:A:156:ASP:OD1	1:A:769:LYS:NZ	2.49	0.45
1:A:189:ASN:O	1:A:191:ASN:N	2.50	0.45
1:A:368:PRO:HB3	1:A:409:ALA:HB1	1.98	0.45
1:A:917:THR:O	1:A:919:ARG:N	2.49	0.45
1:B:27:ILE:HG13	1:B:28:LEU:N	2.31	0.45
1:B:775:SER:OG	1:B:789:TRP:HZ2	1.99	0.45
1:C:518:ARG:HA	1:C:518:ARG:NH2	2.30	0.45
1:C:706:ALA:CB	1:C:716:VAL:HG21	2.46	0.45
1:C:894:SER:O	1:C:898:PRO:CD	2.64	0.45
1:C:934:THR:O	1:C:935:ILE:C	2.59	0.45
1:A:626:ILE:HD13	1:A:626:ILE:HA	1.77	0.45
1:A:651:ALA:O	1:A:652:THR:C	2.58	0.45
1:A:799:VAL:HG13	1:A:800:PRO:HD2	1.97	0.45
1:B:78:MET:HB3	1:B:92:LEU:HD13	1.98	0.45
1:B:235:ILE:N	1:B:235:ILE:CD1	2.78	0.45
1:C:344:LEU:HD23	1:C:399:VAL:CG2	2.47	0.45
1:A:391:ASN:O	1:A:392:THR:C	2.58	0.45
1:A:841:MET:O	1:A:845:GLU:HG3	2.17	0.45
1:B:70:ASN:ND2	1:B:70:ASN:N	2.65	0.45
1:B:537:SER:HA	1:B:540:ARG:NH2	2.31	0.45
1:B:930:GLY:O	1:B:934:THR:HG23	2.17	0.45
1:C:39:ALA:HB2	1:C:673:GLU:HG2	1.97	0.45
1:C:189:ASN:ND2	1:C:191:ASN:H	2.14	0.45
1:C:713:LEU:HD12	1:C:835:LYS:N	2.31	0.45
1:C:843:LEU:O	1:C:847:LEU:HD23	2.17	0.45
1:A:105:VAL:HG21	1:B:105:VAL:HG13	1.98	0.45
1:A:713:LEU:CD2	1:A:714:THR:H	2.30	0.45
1:A:951:ASP:C	1:A:953:MET:H	2.25	0.45
1:B:49:TYR:HE1	1:B:60:THR:HG21	1.82	0.45
1:B:406:VAL:O	1:B:407:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:ALA:C	1:B:637:ARG:H	2.24	0.45
1:C:658:ILE:C	1:C:659:LYS:HD2	2.42	0.45
1:C:888:LEU:HD13	1:C:901:VAL:HG23	1.99	0.45
1:C:934:THR:O	1:C:936:GLY:N	2.50	0.45
1:A:298:ASN:O	1:A:302:THR:HG23	2.16	0.45
1:A:355:MET:HB3	1:A:365:THR:HB	1.97	0.45
1:B:193:LEU:HD22	1:B:198:LEU:O	2.17	0.45
1:B:318:PRO:HD2	1:B:321:LEU:HD22	1.99	0.45
1:B:462:SER:OG	1:B:865:GLN:CG	2.64	0.45
1:C:398:MET:HE3	1:C:473:THR:CG2	2.46	0.45
1:C:541:TYR:C	1:C:543:VAL:N	2.73	0.45
1:A:579:PRO:O	1:A:580:ALA:O	2.34	0.45
1:B:183:ALA:O	1:B:184:MET:C	2.59	0.45
1:B:463:THR:HG21	1:B:869:SER:CB	2.39	0.45
1:B:945:ILE:HD11	1:B:1022:VAL:HB	1.99	0.45
1:B:966:ASP:O	1:B:970:MET:CG	2.65	0.45
1:C:77:TYR:N	1:C:77:TYR:CD2	2.85	0.45
1:C:160:ALA:HA	1:C:767:ARG:NE	2.32	0.45
1:C:666:PHE:CZ	2:C:2002:RFP:H28C	2.52	0.45
1:A:252:LYS:HB3	1:A:260:VAL:HB	1.99	0.45
1:A:682:PHE:CZ	1:A:857:TYR:CB	2.98	0.45
1:A:713:LEU:HB2	1:A:832:ALA:N	2.31	0.45
1:B:44:THR:OG1	1:B:132:SER:CB	2.65	0.45
1:B:169:THR:HG22	1:B:170:SER:N	2.31	0.45
1:B:326:PRO:HB2	1:B:327:TYR:H	1.63	0.45
1:C:732:ASP:O	1:C:733:GLN:C	2.58	0.45
1:A:219:LEU:HD23	1:B:754:TRP:CZ3	2.52	0.45
1:A:681:ASP:HB3	1:A:860:THR:O	2.16	0.45
1:A:843:LEU:HD22	1:A:843:LEU:C	2.42	0.45
1:B:13:TRP:CE3	1:B:488:LEU:HD21	2.52	0.45
1:B:651:ALA:O	1:B:655:PHE:HD2	1.99	0.45
1:B:680:PHE:O	1:B:828:LEU:HD23	2.17	0.45
1:C:35:TYR:CE1	1:C:671:ILE:HG12	2.51	0.45
1:C:44:THR:HB	1:C:91:THR:HB	1.99	0.45
1:C:78:MET:O	1:C:78:MET:HG3	2.16	0.45
1:C:350:LEU:C	1:C:352:PHE:N	2.75	0.45
1:C:354:VAL:HG21	1:C:980:LEU:O	2.17	0.45
1:C:548:ILE:HD13	1:C:1017:LEU:HD21	1.98	0.45
1:C:577:GLN:HG2	2:C:2002:RFP:H391	1.99	0.45
1:C:591:LEU:HD23	1:C:613:ASN:HB2	1.98	0.45
1:C:914:LEU:O	1:C:915:ALA:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PRO:C	1:A:492:LEU:N	2.74	0.45
1:B:455:PRO:HG3	1:B:880:SER:HA	1.99	0.45
1:C:365:THR:O	1:C:365:THR:CG2	2.66	0.45
1:A:103:ALA:O	1:A:107:VAL:HG23	2.17	0.44
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.51	0.44
1:A:808:ARG:HG2	1:A:808:ARG:HH11	1.83	0.44
1:B:240:LEU:HD22	1:B:245:GLU:OE1	2.16	0.44
1:B:983:ILE:CD1	1:B:1012:VAL:HG13	2.47	0.44
1:C:53:ASP:O	1:C:54:ALA:CB	2.65	0.44
1:A:688:ALA:C	1:A:690:LEU:N	2.76	0.44
1:B:213:GLN:HE21	1:B:213:GLN:HB2	1.69	0.44
1:B:561:SER:HB3	1:B:563:PHE:CE1	2.52	0.44
1:B:680:PHE:CD1	1:B:859:TRP:CZ3	3.03	0.44
1:B:695:LEU:HD12	1:B:825:MET:CE	2.46	0.44
1:B:966:ASP:O	1:B:970:MET:HG2	2.17	0.44
1:C:172:VAL:O	1:C:172:VAL:HG12	2.18	0.44
1:C:454:VAL:N	1:C:455:PRO:HD2	2.32	0.44
1:C:971:ARG:HB3	1:C:975:ILE:HD13	2.00	0.44
1:A:416:VAL:O	1:A:420:MET:HB2	2.17	0.44
1:A:1022:VAL:HA	1:A:1025:PHE:CD1	2.52	0.44
1:B:83:ASP:OD1	1:B:87:THR:HB	2.17	0.44
1:C:10:ILE:HG12	1:C:11:PHE:H	1.82	0.44
1:C:314:GLU:N	1:C:315:PRO:CD	2.80	0.44
1:C:415:ASN:OD1	1:C:418:ARG:NE	2.42	0.44
1:A:339:GLU:O	1:A:341:VAL:N	2.49	0.44
1:A:413:VAL:HG23	1:A:493:CYS:SG	2.57	0.44
1:B:187:TRP:O	1:B:266:ALA:HB1	2.17	0.44
1:B:314:GLU:OE2	1:B:323:ILE:HD12	2.18	0.44
1:B:669:PRO:CB	1:B:862:MET:HE2	2.47	0.44
1:C:696:THR:O	1:C:699:ARG:HG3	2.17	0.44
1:C:945:ILE:C	1:C:947:GLU:N	2.62	0.44
1:A:166:ILE:O	1:A:172:VAL:HG21	2.17	0.44
1:A:884:VAL:O	1:A:888:LEU:HB2	2.17	0.44
1:A:901:VAL:HG13	1:A:942:ALA:HB3	1.99	0.44
1:B:22:ALA:C	1:B:23:GLY:O	2.60	0.44
1:B:49:TYR:CE1	1:B:60:THR:HG21	2.52	0.44
1:B:72:ILE:O	1:B:73:ASP:C	2.60	0.44
1:B:231:ASN:HD22	1:B:232:ALA:N	2.15	0.44
1:C:203:VAL:HG13	1:C:262:LEU:HD11	1.98	0.44
1:C:653:ARG:O	1:C:655:PHE:O	2.36	0.44
1:A:926:TYR:CE1	1:A:999:ALA:HB1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:THR:C	1:A:936:GLY:H	2.25	0.44
1:B:166:ILE:HA	1:B:169:THR:OG1	2.17	0.44
1:B:192:GLU:OE1	1:B:196:PHE:HE2	1.99	0.44
1:B:289:LEU:CD1	1:B:289:LEU:N	2.79	0.44
1:B:332:PHE:HB2	1:B:569:GLN:O	2.18	0.44
1:B:356:TYR:O	1:B:358:PHE:N	2.47	0.44
1:B:402:ILE:HD12	1:B:402:ILE:HA	1.80	0.44
1:B:597:TYR:CD2	1:B:597:TYR:C	2.95	0.44
1:B:673:GLU:HG2	1:B:861:GLY:HA2	2.00	0.44
1:C:92:LEU:HD12	1:C:92:LEU:H	1.83	0.44
1:C:102:ILE:O	1:C:103:ALA:C	2.60	0.44
1:C:307:ARG:HE	1:C:307:ARG:HB3	1.57	0.44
1:C:669:PRO:O	1:C:670:ALA:C	2.60	0.44
1:A:255:GLN:O	1:A:256:ASP:CB	2.65	0.44
1:A:454:VAL:C	1:A:456:MET:N	2.76	0.44
1:A:973:ARG:O	1:A:974:PRO:C	2.60	0.44
1:C:5:PHE:CE2	1:C:11:PHE:CD2	2.96	0.44
1:C:394:THR:HG22	1:C:395:MET:CE	2.47	0.44
1:C:415:ASN:ND2	1:C:434:SER:HB2	2.33	0.44
1:A:76:MET:HE3	1:A:864:TYR:CE2	2.53	0.44
1:A:375:VAL:CG2	1:A:481:SER:HA	2.45	0.44
1:A:525:HIS:O	1:A:528:THR:HG22	2.18	0.44
1:A:644:VAL:C	1:A:646:ALA:N	2.76	0.44
1:A:731:ILE:HG12	1:A:746:ILE:HG21	2.00	0.44
1:B:20:MET:CG	1:B:374:VAL:HA	2.48	0.44
1:C:687:GLN:HE21	1:C:687:GLN:HB3	1.48	0.44
1:A:235:ILE:HG22	1:A:235:ILE:O	2.16	0.44
1:A:490:PRO:C	1:A:492:LEU:H	2.25	0.44
1:A:907:LEU:HG	1:A:1017:LEU:HD22	2.00	0.44
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.53	0.44
1:B:747:ASN:C	1:B:749:THR:H	2.24	0.44
1:B:878:ALA:O	1:B:882:ILE:HG12	2.18	0.44
1:C:220:GLY:HA3	1:C:231:ASN:HD22	1.82	0.44
1:C:427:PRO:HB3	1:C:498:LYS:HD2	1.99	0.44
1:C:1020:PHE:C	1:C:1023:PRO:HD2	2.43	0.44
1:B:5:PHE:HB3	1:B:12:ALA:HB2	2.00	0.43
1:B:33:ALA:O	1:B:391:ASN:HA	2.18	0.43
1:B:143:ILE:CD1	1:B:322:LYS:HB3	2.48	0.43
1:B:190:PRO:HB3	1:B:789:TRP:CD2	2.53	0.43
1:B:562:SER:O	1:B:924:ASP:HA	2.18	0.43
1:B:674:LEU:HD23	1:B:674:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:ALA:HA	1:B:713:LEU:HD22	2.00	0.43
1:C:579:PRO:O	1:C:580:ALA:O	2.36	0.43
1:A:138:MET:HE3	1:A:306:ILE:HD12	1.99	0.43
1:A:347:ALA:HB3	1:A:402:ILE:HD13	2.00	0.43
1:A:882:ILE:O	1:A:886:LEU:HB2	2.18	0.43
1:B:447:MET:HE1	1:B:887:CYS:O	2.18	0.43
1:B:932:LEU:HA	1:B:935:ILE:HD12	2.00	0.43
1:C:106:GLN:O	1:C:107:VAL:C	2.59	0.43
1:C:188:MET:CE	1:C:193:LEU:HD11	2.44	0.43
1:C:368:PRO:CD	1:C:369:THR:H	2.30	0.43
1:C:372:VAL:HG12	1:C:373:PRO:CD	2.34	0.43
1:C:931:LEU:O	1:C:935:ILE:HD13	2.18	0.43
1:A:747:ASN:HD21	1:C:237:GLN:HE22	1.66	0.43
1:C:265:VAL:O	1:C:266:ALA:CB	2.63	0.43
1:C:319:SER:OG	1:C:320:GLY:N	2.39	0.43
1:C:445:ILE:O	1:C:448:VAL:N	2.51	0.43
1:C:904:VAL:O	1:C:905:VAL:C	2.61	0.43
1:A:184:MET:HB3	1:A:771:VAL:HG13	2.00	0.43
1:A:578:LEU:HD11	1:A:590:VAL:HG21	1.99	0.43
1:B:222:THR:CG2	1:B:223:PRO:HD3	2.48	0.43
1:B:367:ILE:HD11	1:B:496:MET:HB2	2.00	0.43
1:B:959:GLY:O	1:B:960:LEU:C	2.62	0.43
1:C:683:GLU:HG3	1:C:819:TYR:CD2	2.52	0.43
1:C:815:ARG:NH2	2:C:2002:RFP:H302	2.34	0.43
1:C:982:PHE:HD2	1:C:982:PHE:HA	1.77	0.43
1:A:338:HIS:O	1:A:341:VAL:HG12	2.18	0.43
1:A:406:VAL:O	1:A:408:ASP:N	2.51	0.43
1:A:781:MET:HE2	1:C:225:VAL:N	2.31	0.43
1:B:97:GLY:O	1:B:98:THR:O	2.37	0.43
1:B:144:ASN:ND2	1:B:149:MET:H	2.16	0.43
1:B:703:LEU:HD21	1:B:718:PRO:HD3	2.01	0.43
1:A:742:SER:OG	1:A:745:ASP:HB2	2.19	0.43
1:A:754:TRP:CE3	1:A:780:ARG:HB2	2.53	0.43
1:A:817:GLU:HB2	1:A:824:SER:O	2.18	0.43
1:A:894:SER:OG	1:A:898:PRO:HD2	2.19	0.43
1:C:367:ILE:N	1:C:368:PRO:HD3	2.33	0.43
1:A:60:THR:HG23	1:A:119:PRO:CG	2.42	0.43
1:A:254:ASN:CG	1:A:258:SER:OG	2.61	0.43
1:A:819:TYR:H	1:A:824:SER:HB3	1.83	0.43
1:A:910:ILE:O	1:A:1013:THR:OG1	2.34	0.43
1:B:166:ILE:C	1:B:168:ARG:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:HG11	1:C:778:LYS:HB3	2.00	0.43
1:B:356:TYR:C	1:B:358:PHE:N	2.77	0.43
1:B:606:VAL:CG1	1:B:607:GLU:N	2.82	0.43
1:B:699:ARG:C	1:B:701:GLN:N	2.75	0.43
1:C:229:GLN:O	1:C:230:LEU:HB3	2.17	0.43
1:C:713:LEU:O	1:C:830:GLN:O	2.37	0.43
1:C:792:ARG:HG3	1:C:796:GLY:HA2	2.00	0.43
1:A:76:MET:HE3	1:A:864:TYR:HE2	1.84	0.43
1:A:187:TRP:O	1:A:188:MET:O	2.37	0.43
1:A:636:ASP:O	1:A:638:PRO:HD3	2.18	0.43
1:A:848:ALA:HA	1:A:851:LEU:HD12	2.01	0.43
1:B:145:THR:HG23	1:B:320:GLY:CA	2.48	0.43
1:B:449:LEU:HD23	1:B:478:MET:SD	2.59	0.43
1:B:544:LEU:HB3	1:B:1021:PHE:HZ	1.82	0.43
1:C:34:GLN:CG	1:C:333:VAL:HG21	2.48	0.43
1:C:894:SER:C	1:C:896:SER:N	2.76	0.43
1:A:29:LYS:CG	1:A:30:LEU:H	2.32	0.43
1:A:899:PHE:O	1:A:903:LEU:HG	2.19	0.43
1:B:119:PRO:HB2	1:B:122:VAL:HG23	2.01	0.43
1:B:183:ALA:N	1:B:271:GLY:O	2.48	0.43
1:B:952:LEU:HG	1:B:956:GLU:OE1	2.18	0.43
1:C:247:GLY:CA	1:C:263:ARG:HD3	2.49	0.43
1:C:303:ALA:O	1:C:304:ALA:C	2.61	0.43
1:C:713:LEU:CD2	1:C:830:GLN:O	2.65	0.43
1:A:352:PHE:HD1	1:A:353:LEU:HD12	1.84	0.43
1:B:675:GLY:O	1:B:676:THR:C	2.62	0.43
1:A:166:ILE:HD13	1:A:166:ILE:N	2.34	0.42
1:B:94:PHE:CB	1:B:98:THR:HG21	2.41	0.42
1:B:157:TYR:HA	1:B:161:ASN:ND2	2.34	0.42
1:B:169:THR:HB	1:B:172:VAL:HG21	2.00	0.42
1:B:962:GLU:O	1:B:966:ASP:HB2	2.18	0.42
1:C:18:ILE:O	1:C:19:ILE:C	2.60	0.42
1:C:66:GLU:HA	1:C:69:MET:HB2	2.00	0.42
1:C:186:ILE:O	1:C:186:ILE:CG2	2.66	0.42
1:C:241:THR:HG22	1:C:245:GLU:OE2	2.19	0.42
1:C:341:VAL:O	1:C:344:LEU:HB3	2.19	0.42
1:C:697:GLN:O	1:C:700:ASN:HB2	2.19	0.42
1:A:53:ASP:O	1:A:54:ALA:C	2.61	0.42
1:A:195:LYS:C	1:A:197:GLN:H	2.27	0.42
1:A:758:TYR:HB2	1:A:772:TYR:CE2	2.54	0.42
1:B:790:TYR:HD1	1:B:800:PRO:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASP:CG	1:C:182:TYR:CD2	2.96	0.42
1:C:731:ILE:HG12	1:C:746:ILE:HG21	2.01	0.42
1:A:149:MET:HE1	1:A:321:LEU:HD13	2.00	0.42
1:A:335:ILE:O	1:A:339:GLU:HG3	2.19	0.42
1:A:426:PRO:HB3	1:A:427:PRO:HD2	2.00	0.42
1:B:314:GLU:N	1:B:315:PRO:HD3	2.34	0.42
1:B:393:LEU:HD13	1:B:466:ILE:HG23	2.01	0.42
1:B:708:LYS:O	1:B:708:LYS:HG2	2.19	0.42
1:B:828:LEU:HB3	1:B:829:GLY:H	1.76	0.42
1:B:961:ILE:HG22	1:B:961:ILE:O	2.19	0.42
1:C:131:LYS:O	1:C:131:LYS:HG3	2.18	0.42
1:C:873:ALA:C	1:C:875:SER:N	2.74	0.42
1:C:886:LEU:O	1:C:890:ALA:HB2	2.19	0.42
1:A:571:VAL:HG12	1:A:630:SER:HB3	2.00	0.42
1:A:617:PHE:O	1:A:618:ALA:HB3	2.20	0.42
1:A:653:ARG:O	1:A:654:ALA:C	2.62	0.42
1:A:655:PHE:O	1:A:658:ILE:HG13	2.19	0.42
1:B:188:MET:HA	1:B:188:MET:HE2	2.00	0.42
1:B:372:VAL:HG22	1:B:373:PRO:HD3	2.00	0.42
1:B:897:ILE:N	1:B:898:PRO:CD	2.83	0.42
1:C:591:LEU:HD13	1:C:591:LEU:HA	1.90	0.42
1:C:767:ARG:CG	1:C:767:ARG:NH1	2.69	0.42
1:A:355:MET:HG2	1:A:365:THR:HA	2.02	0.42
1:B:250:LEU:HD11	1:B:253:VAL:HG23	2.01	0.42
1:B:780:ARG:O	1:B:780:ARG:HG2	2.19	0.42
1:B:888:LEU:C	1:B:890:ALA:N	2.72	0.42
1:C:331:PRO:HG2	1:C:332:PHE:H	1.85	0.42
1:A:323:ILE:O	1:A:323:ILE:HG13	2.20	0.42
1:A:655:PHE:O	1:A:657:GLN:N	2.41	0.42
1:A:702:LEU:HB2	1:A:851:LEU:HD11	2.01	0.42
1:B:990:VAL:HG13	1:B:1005:THR:OG1	2.19	0.42
1:C:30:LEU:HD21	1:C:384:ALA:HA	2.01	0.42
1:C:169:THR:O	1:C:170:SER:C	2.61	0.42
1:C:372:VAL:HG21	1:C:406:VAL:HG22	2.02	0.42
1:C:395:MET:C	1:C:397:GLY:N	2.77	0.42
1:C:466:ILE:HD13	1:C:466:ILE:N	2.35	0.42
1:A:141:GLY:N	1:A:324:VAL:O	2.46	0.42
1:A:187:TRP:HA	1:A:774:MET:O	2.19	0.42
1:A:400:LEU:HD12	1:A:400:LEU:O	2.20	0.42
1:A:780:ARG:NH1	1:A:780:ARG:CG	2.82	0.42
1:B:111:LEU:C	1:B:113:LEU:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:THR:O	1:B:347:ALA:HB2	2.20	0.42
1:B:602:GLU:C	1:B:604:ASN:H	2.28	0.42
1:B:778:LYS:C	1:B:780:ARG:N	2.72	0.42
1:C:644:VAL:HG12	1:C:667:ASN:HB2	2.02	0.42
1:A:191:ASN:C	1:A:193:LEU:N	2.78	0.42
1:A:211:ASN:CG	1:A:211:ASN:O	2.62	0.42
1:A:472:ILE:O	1:A:473:THR:C	2.61	0.42
1:A:565:PRO:HG2	1:A:999:ALA:HA	2.01	0.42
1:A:701:GLN:HE21	1:A:701:GLN:HB2	1.61	0.42
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.20	0.42
1:B:568:ASP:HA	1:B:644:VAL:CG2	2.49	0.42
1:B:692:HIS:O	1:B:692:HIS:ND1	2.53	0.42
1:B:701:GLN:HB3	1:B:851:LEU:CD1	2.50	0.42
1:B:972:LEU:HD21	1:B:1019:ILE:HD12	2.02	0.42
1:C:672:VAL:HG13	1:C:675:GLY:N	2.34	0.42
1:C:869:SER:HB2	1:C:870:GLY:H	1.71	0.42
1:C:941:ASN:HA	1:C:944:LEU:HD12	2.02	0.42
1:C:988:PRO:O	1:C:989:LEU:C	2.63	0.42
1:A:203:VAL:O	1:A:207:ILE:HG13	2.20	0.42
1:A:872:GLN:O	1:A:873:ALA:C	2.63	0.42
1:A:897:ILE:HD11	1:A:1030:ARG:HD3	2.01	0.42
1:B:118:LEU:O	1:B:119:PRO:C	2.63	0.42
1:B:204:ILE:HG23	1:B:759:VAL:HG13	2.02	0.42
1:B:216:ALA:HB2	1:B:236:ALA:HB2	2.02	0.42
1:B:425:LEU:HB3	1:B:498:LYS:C	2.45	0.42
1:C:131:LYS:C	1:C:295:THR:HG22	2.44	0.42
1:C:137:LEU:N	1:C:291:ILE:O	2.52	0.42
1:C:577:GLN:O	1:C:661:ALA:HB1	2.19	0.42
1:A:36:PRO:HG3	1:A:469:GLN:CD	2.45	0.42
1:A:49:TYR:O	1:A:52:ALA:HB2	2.20	0.42
1:A:295:THR:O	1:A:295:THR:HG22	2.20	0.42
1:A:367:ILE:HG13	1:A:368:PRO:HD3	2.02	0.42
1:A:442:LEU:C	1:A:444:GLY:N	2.78	0.42
1:A:589:LYS:HA	1:A:589:LYS:HD3	1.81	0.42
1:B:704:ALA:O	1:B:705:GLU:CB	2.68	0.42
1:B:764:ASP:C	1:B:766:GLY:N	2.78	0.42
1:C:453:PHE:C	1:C:455:PRO:HD2	2.45	0.42
1:C:574:THR:HB	1:C:627:ALA:HB3	2.02	0.42
1:C:668:LEU:H	1:C:668:LEU:HD23	1.85	0.42
1:C:897:ILE:O	1:C:900:SER:OG	2.31	0.42
1:A:20:MET:HG3	1:A:374:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:OE1	1:C:767:ARG:HA	2.20	0.41
1:A:713:LEU:CG	1:A:714:THR:H	2.33	0.41
1:B:391:ASN:OD1	1:B:394:THR:N	2.35	0.41
1:B:516:PHE:CG	1:B:517:ASN:N	2.84	0.41
1:C:3:ASN:C	1:C:5:PHE:N	2.78	0.41
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.55	0.41
1:C:204:ILE:O	1:C:205:THR:C	2.63	0.41
1:C:240:LEU:HB3	1:C:245:GLU:HB2	2.02	0.41
1:C:395:MET:HE2	1:C:395:MET:HA	2.02	0.41
1:C:426:PRO:HA	1:C:427:PRO:HD3	1.64	0.41
1:A:72:ILE:HG23	1:A:106:GLN:HE21	1.84	0.41
1:A:282:ASN:HD22	1:A:282:ASN:HA	1.62	0.41
1:A:578:LEU:O	1:A:623:ASN:ND2	2.53	0.41
1:A:895:TRP:HZ2	1:C:13:TRP:HE3	1.67	0.41
1:B:34:GLN:HE21	1:B:332:PHE:HE2	1.68	0.41
1:B:38:ILE:HG23	1:B:462:SER:HB2	2.01	0.41
1:B:186:ILE:HD13	1:B:262:LEU:HD11	2.02	0.41
1:B:204:ILE:H	1:B:204:ILE:HG12	1.74	0.41
1:B:280:GLU:HG2	1:B:611:ALA:HB3	2.01	0.41
1:B:367:ILE:HG13	1:B:492:LEU:CB	2.28	0.41
1:B:700:ASN:O	1:B:704:ALA:CB	2.68	0.41
1:B:852:PRO:HA	1:B:855:VAL:HB	2.02	0.41
1:B:983:ILE:HD12	1:B:1012:VAL:CG1	2.50	0.41
1:C:284:GLN:HE21	1:C:284:GLN:HB2	1.65	0.41
1:C:388:PHE:N	1:C:388:PHE:CD1	2.87	0.41
1:A:340:VAL:O	1:A:344:LEU:HB2	2.20	0.41
1:A:575:MET:HG2	1:A:626:ILE:HD11	2.02	0.41
1:A:818:ARG:NH2	1:A:821:GLY:O	2.52	0.41
1:A:983:ILE:HG13	1:A:984:LEU:N	2.35	0.41
1:A:1029:VAL:HG12	1:A:1030:ARG:N	2.33	0.41
1:B:58:GLN:HE22	1:B:818:ARG:NH1	2.18	0.41
1:B:586:ARG:O	1:B:587:THR:C	2.62	0.41
1:C:445:ILE:O	1:C:448:VAL:HG12	2.19	0.41
1:A:194:ASN:ND2	1:A:790:TYR:CE2	2.88	0.41
1:A:538:THR:C	1:A:540:ARG:H	2.27	0.41
1:B:10:ILE:H	1:B:10:ILE:HG13	1.62	0.41
1:B:154:ILE:HD11	1:B:286:ALA:HA	2.02	0.41
1:B:185:ARG:HH22	1:B:774:MET:CE	2.29	0.41
1:B:216:ALA:HB3	1:B:234:ILE:O	2.21	0.41
1:B:396:PHE:CD2	1:B:1003:VAL:HG21	2.54	0.41
1:C:34:GLN:HA	1:C:333:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2002:RFP:O4	2:C:2002:RFP:O12	2.35	0.41
1:A:6:ILE:HG21	1:A:490:PRO:HB2	2.02	0.41
1:A:89:GLN:HE21	1:A:89:GLN:HB2	1.62	0.41
1:A:301:ASP:O	1:A:305:ALA:N	2.49	0.41
1:A:660:ASP:O	1:A:661:ALA:HB2	2.18	0.41
1:A:836:SER:O	1:A:839:GLU:HG2	2.21	0.41
1:A:895:TRP:HZ2	1:C:13:TRP:CE3	2.38	0.41
1:A:983:ILE:C	1:A:985:GLY:H	2.29	0.41
1:B:564:LEU:HA	1:B:565:PRO:HD3	1.71	0.41
1:B:669:PRO:HB2	1:B:862:MET:CE	2.50	0.41
1:B:680:PHE:HZ	1:B:716:VAL:HG22	1.84	0.41
1:B:901:VAL:C	1:B:903:LEU:H	2.29	0.41
1:B:1017:LEU:HD12	1:B:1017:LEU:N	2.35	0.41
1:C:2:PRO:O	1:C:6:ILE:HG12	2.21	0.41
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.83	0.41
1:C:456:MET:CA	1:C:459:PHE:HE1	2.28	0.41
1:C:467:TYR:CZ	1:C:925:VAL:HG12	2.56	0.41
1:C:748:THR:O	1:C:752:ALA:CB	2.69	0.41
1:C:901:VAL:HG11	1:C:943:ILE:HA	2.01	0.41
1:A:178:PHE:HB2	1:A:288:GLY:C	2.46	0.41
1:A:183:ALA:N	1:A:271:GLY:O	2.53	0.41
1:A:200:PRO:CD	1:A:749:THR:HG23	2.51	0.41
1:A:301:ASP:C	1:A:303:ALA:N	2.78	0.41
1:A:685:ILE:HD11	1:A:819:TYR:HD1	1.86	0.41
1:A:739:LEU:C	1:A:741:VAL:H	2.28	0.41
1:B:14:VAL:HG21	1:C:886:LEU:O	2.21	0.41
1:B:121:GLU:H	1:B:121:GLU:HG2	1.42	0.41
1:B:317:PHE:HB3	1:B:321:LEU:HB3	2.03	0.41
1:B:462:SER:O	1:B:466:ILE:HG12	2.20	0.41
1:C:34:GLN:O	1:C:392:THR:HG23	2.20	0.41
1:C:92:LEU:HD12	1:C:92:LEU:N	2.35	0.41
1:C:189:ASN:HA	1:C:190:PRO:HD3	1.80	0.41
1:C:592:ASN:O	1:C:593:GLU:CB	2.65	0.41
1:A:298:ASN:C	1:A:300:LEU:N	2.77	0.41
1:A:579:PRO:CG	1:A:660:ASP:HB2	2.47	0.41
1:A:733:GLN:HE22	1:A:743:ILE:HG12	1.85	0.41
1:B:200:PRO:O	1:B:204:ILE:HG12	2.20	0.41
1:A:186:ILE:HD13	1:A:262:LEU:HD21	2.02	0.41
1:A:845:GLU:O	1:A:848:ALA:HB3	2.21	0.41
1:A:895:TRP:HA	1:A:895:TRP:CE3	2.55	0.41
1:B:34:GLN:HB2	1:B:333:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ILE:HB	1:B:90:ILE:HB	2.03	0.41
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.55	0.41
1:B:213:GLN:HE21	1:B:239:ARG:CD	2.30	0.41
1:B:527:TYR:HA	1:B:530:SER:CB	2.49	0.41
1:B:790:TYR:CE1	1:B:800:PRO:HB3	2.55	0.41
1:B:899:PHE:O	1:B:903:LEU:HG	2.21	0.41
1:C:83:ASP:HB3	1:C:85:THR:H	1.86	0.41
1:C:262:LEU:HD23	1:C:268:ILE:HD11	2.03	0.41
1:C:736:ALA:C	1:C:738:ALA:N	2.79	0.41
1:C:801:PHE:CD1	1:C:804:PHE:CE1	3.09	0.41
1:A:294:ALA:O	1:A:295:THR:CB	2.69	0.41
1:A:467:TYR:CE1	1:A:925:VAL:HG13	2.56	0.41
1:A:516:PHE:O	1:A:519:MET:N	2.50	0.41
1:A:519:MET:O	1:A:523:SER:HB2	2.20	0.41
1:A:607:GLU:HB3	1:A:630:SER:O	2.20	0.41
1:B:111:LEU:C	1:B:113:LEU:H	2.28	0.41
1:B:318:PRO:O	1:B:319:SER:C	2.63	0.41
1:B:973:ARG:O	1:B:977:MET:HG2	2.21	0.41
1:C:1:MET:CB	1:C:2:PRO:CD	2.97	0.41
1:C:5:PHE:HE2	1:C:11:PHE:HD2	1.60	0.41
1:C:218:GLN:HG3	1:C:233:SER:HA	2.03	0.41
1:C:354:VAL:HG11	1:C:980:LEU:C	2.46	0.41
1:C:470:PHE:O	1:C:471:SER:C	2.63	0.41
1:C:832:ALA:CB	1:C:833:PRO:CD	2.93	0.41
1:A:753:ALA:C	1:A:775:SER:HB3	2.46	0.41
1:B:686:ASP:HB3	1:B:823:PRO:HG2	2.01	0.41
1:B:723:ASP:O	1:B:724:THR:HB	2.21	0.41
1:B:908:GLY:CA	1:B:1014:ALA:HB2	2.50	0.41
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	2.03	0.41
1:B:948:PHE:HB2	1:B:971:ARG:NH2	2.36	0.41
1:C:474:ILE:O	1:C:476:SER:O	2.38	0.41
1:A:83:ASP:HA	1:A:815:ARG:HA	2.03	0.40
1:A:139:VAL:O	1:A:326:PRO:HD2	2.21	0.40
1:A:418:ARG:NH2	1:A:970:MET:C	2.78	0.40
1:A:516:PHE:O	1:A:518:ARG:N	2.54	0.40
1:B:356:TYR:CD2	1:B:365:THR:HG21	2.56	0.40
1:C:34:GLN:HB2	1:C:35:TYR:CD1	2.55	0.40
1:C:144:ASN:HD22	1:C:149:MET:H	1.66	0.40
1:C:325:TYR:O	1:C:326:PRO:O	2.39	0.40
1:C:947:GLU:O	1:C:948:PHE:C	2.64	0.40
1:A:150:THR:O	1:A:154:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:C	1:A:408:ASP:N	2.79	0.40
1:A:617:PHE:O	1:A:618:ALA:CB	2.69	0.40
1:A:633:ASP:O	1:A:636:ASP:N	2.46	0.40
1:A:659:LYS:CG	1:A:660:ASP:N	2.83	0.40
1:B:203:VAL:O	1:B:204:ILE:C	2.64	0.40
1:A:418:ARG:HG2	1:A:970:MET:HE3	2.03	0.40
1:A:559:LEU:HA	1:A:560:PRO:HD3	1.92	0.40
1:A:666:PHE:CD1	1:A:666:PHE:N	2.90	0.40
1:A:759:VAL:HG12	1:A:760:ASN:N	2.37	0.40
1:A:795:ASP:OD1	1:A:795:ASP:C	2.65	0.40
1:B:187:TRP:C	1:B:266:ALA:HB1	2.47	0.40
1:B:346:GLU:HG3	1:B:988:PRO:HG3	2.03	0.40
1:B:468:ARG:O	1:B:469:GLN:C	2.63	0.40
1:B:632:LYS:O	1:B:633:ASP:O	2.40	0.40
1:B:705:GLU:O	1:B:708:LYS:N	2.55	0.40
1:C:203:VAL:HG13	1:C:262:LEU:CD1	2.51	0.40
1:C:220:GLY:HA2	1:C:228:GLN:HE21	1.84	0.40
1:C:445:ILE:O	1:C:446:ALA:C	2.64	0.40
1:C:610:PHE:HB3	1:C:628:PHE:HB2	2.04	0.40
1:C:885:PHE:CE2	1:C:899:PHE:CE1	3.09	0.40
1:A:38:ILE:C	1:A:38:ILE:HD12	2.46	0.40
1:A:140:VAL:HG12	1:A:141:GLY:N	2.37	0.40
1:A:169:THR:CG2	1:A:309:GLU:HG3	2.52	0.40
1:A:281:PHE:CZ	1:A:608:SER:HB2	2.57	0.40
1:A:456:MET:HG2	1:A:471:SER:HB2	2.04	0.40
1:A:707:ALA:O	1:A:710:PRO:CD	2.66	0.40
1:B:110:LYS:HD2	1:B:110:LYS:HA	1.92	0.40
1:B:445:ILE:HD11	1:B:944:LEU:HD21	2.01	0.40
1:B:519:MET:C	1:B:521:GLU:H	2.28	0.40
1:B:703:LEU:H	1:B:703:LEU:HD12	1.85	0.40
1:C:226:LYS:HB3	1:C:227:GLY:H	1.74	0.40
1:C:754:TRP:CE3	1:C:780:ARG:HB2	2.57	0.40
1:C:1016:VAL:HG23	1:C:1017:LEU:H	1.86	0.40
1:A:658:ILE:HG22	1:A:659:LYS:H	1.86	0.40
1:A:704:ALA:C	1:A:706:ALA:H	2.29	0.40
1:B:192:GLU:OE1	1:B:196:PHE:CE2	2.74	0.40
1:B:450:SER:OG	1:B:478:MET:HB2	2.20	0.40
1:B:576:VAL:HG11	1:B:591:LEU:HD22	2.02	0.40
1:B:594:VAL:HA	1:B:655:PHE:CE1	2.56	0.40
1:B:929:VAL:O	1:B:933:THR:OG1	2.36	0.40
1:C:314:GLU:HA	1:C:317:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:PHE:N	1:C:388:PHE:HD1	2.19	0.40
1:C:425:LEU:CB	1:C:426:PRO:HD3	2.47	0.40
1:C:956:GLU:CD	1:C:957:GLY:N	2.76	0.40
1:C:1015:THR:O	1:C:1019:ILE:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1018/1053 (97%)	769 (76%)	174 (17%)	75 (7%)	1	5
1	B	1018/1053 (97%)	742 (73%)	193 (19%)	83 (8%)	0	4
1	C	1018/1053 (97%)	754 (74%)	182 (18%)	82 (8%)	1	4
All	All	3054/3159 (97%)	2265 (74%)	549 (18%)	240 (8%)	1	4

All (240) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	VAL
1	A	188	MET
1	A	239	ARG
1	A	256	ASP
1	A	293	LEU
1	A	295	THR
1	A	357	LEU
1	A	421	ALA
1	A	517	ASN
1	A	534	ILE
1	A	580	ALA
1	A	618	ALA
1	A	659	LYS

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Mol	Chain	Res	Type
1	A	677	ALA
1	A	713	LEU
1	A	832	ALA
1	A	998	GLY
1	A	1008	MET
1	A	1016	VAL
1	B	98	THR
1	B	147	GLY
1	B	184	MET
1	B	222	THR
1	B	270	LEU
1	B	326	PRO
1	B	358	PHE
1	B	517	ASN
1	B	519	MET
1	B	633	ASP
1	B	669	PRO
1	B	676	THR
1	B	705	GLU
1	B	716	VAL
1	B	723	ASP
1	B	733	GLN
1	B	781	MET
1	B	871	ASN
1	C	54	ALA
1	C	223	PRO
1	C	226	LYS
1	C	258	SER
1	C	266	ALA
1	C	319	SER
1	C	326	PRO
1	C	407	ASP
1	C	425	LEU
1	C	427	PRO
1	C	438	ILE
1	C	457	ALA
1	C	463	THR
1	C	532	GLY
1	C	580	ALA
1	C	656	SER
1	C	678	THR
1	C	820	ASN

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Mol	Chain	Res	Type
1	C	825	MET
1	C	869	SER
1	C	946	VAL
1	C	1018	ALA
1	A	5	PHE
1	A	134	SER
1	A	146	ASP
1	A	221	GLY
1	A	236	ALA
1	A	288	GLY
1	A	352	PHE
1	A	407	ASP
1	A	452	VAL
1	A	462	SER
1	A	496	MET
1	A	566	ASP
1	A	634	TRP
1	A	656	SER
1	A	689	GLY
1	A	708	LYS
1	A	787	GLY
1	A	831	ALA
1	A	918	PHE
1	A	951	ASP
1	A	960	LEU
1	A	991	ILE
1	B	37	THR
1	B	53	ASP
1	B	54	ALA
1	B	56	THR
1	B	57	VAL
1	B	227	GLY
1	B	228	GLN
1	B	283	GLY
1	B	361	ASN
1	B	370	ILE
1	B	384	ALA
1	B	453	PHE
1	B	461	GLY
1	B	486	LEU
1	B	557	VAL
1	B	580	ALA

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Mol	Chain	Res	Type
1	B	581	GLY
1	B	613	ASN
1	B	614	GLY
1	B	638	PRO
1	B	656	SER
1	B	671	ILE
1	B	675	GLY
1	B	706	ALA
1	B	765	ARG
1	B	849	SER
1	B	852	PRO
1	B	889	ALA
1	B	953	MET
1	C	216	ALA
1	C	689	GLY
1	C	713	LEU
1	C	720	GLY
1	C	752	ALA
1	C	802	SER
1	C	815	ARG
1	C	832	ALA
1	C	889	ALA
1	C	926	TYR
1	C	935	ILE
1	C	953	MET
1	C	958	LYS
1	C	961	ILE
1	C	993	THR
1	C	1017	LEU
1	A	30	LEU
1	A	53	ASP
1	A	171	GLY
1	A	226	LYS
1	A	282	ASN
1	A	330	THR
1	A	392	THR
1	A	436	GLY
1	A	439	GLN
1	A	443	VAL
1	A	638	PRO
1	A	661	ALA
1	A	914	LEU

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Mol	Chain	Res	Type
1	A	917	THR
1	A	988	PRO
1	A	997	SER
1	B	140	VAL
1	B	269	GLU
1	B	299	ALA
1	B	319	SER
1	B	363	ARG
1	B	385	ALA
1	B	583	THR
1	B	601	LYS
1	B	602	GLU
1	B	672	VAL
1	B	707	ALA
1	B	779	TYR
1	B	851	LEU
1	B	893	GLU
1	B	909	VAL
1	B	921	LEU
1	B	959	GLY
1	C	243	THR
1	C	255	GLN
1	C	368	PRO
1	C	478	MET
1	C	520	PHE
1	C	530	SER
1	C	579	PRO
1	C	602	GLU
1	C	690	LEU
1	C	711	ASP
1	C	721	LEU
1	C	778	LYS
1	C	806	SER
1	C	925	VAL
1	C	994	GLY
1	A	9	PRO
1	A	52	ALA
1	A	184	MET
1	A	193	LEU
1	A	294	ALA
1	A	992	SER
1	B	153	ASP

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Mol	Chain	Res	Type
1	B	618	ALA
1	B	690	LEU
1	B	820	ASN
1	B	997	SER
1	B	1016	VAL
1	C	69	MET
1	C	257	GLY
1	C	351	VAL
1	C	422	GLU
1	C	514	GLY
1	C	516	PHE
1	C	554	TYR
1	C	601	LYS
1	C	671	ILE
1	C	915	ALA
1	C	952	LEU
1	C	965	LEU
1	A	361	ASN
1	A	459	PHE
1	B	126	GLY
1	B	127	VAL
1	B	360	GLN
1	B	603	LYS
1	B	640	GLU
1	C	230	LEU
1	C	372	VAL
1	C	464	GLY
1	C	803	ALA
1	C	982	PHE
1	C	995	ALA
1	A	29	LYS
1	A	192	GLU
1	A	584	GLN
1	A	806	SER
1	A	994	GLY
1	A	1004	GLY
1	B	490	PRO
1	B	542	LEU
1	B	621	GLY
1	B	861	GLY
1	C	86	GLY
1	C	534	ILE

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Mol	Chain	Res	Type
1	C	1005	THR
1	A	15	ILE
1	A	746	ILE
1	A	975	ILE
1	B	783	PRO
1	B	834	GLY
1	B	974	PRO
1	C	539	GLY
1	C	998	GLY
1	A	107	VAL
1	C	743	ILE
1	B	223	PRO
1	C	658	ILE
1	C	756	GLY
1	C	759	VAL
1	C	411	VAL
1	C	716	VAL

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	833/859 (97%)	689 (83%)	144 (17%)	2	8
1	B	833/859 (97%)	686 (82%)	147 (18%)	2	8
1	C	833/859 (97%)	704 (84%)	129 (16%)	2	10
All	All	2499/2577 (97%)	2079 (83%)	420 (17%)	2	9

All (420) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	10	ILE
1	A	25	LEU
1	A	28	LEU
1	A	46	SER

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Mol	Chain	Res	Type
1	A	57	VAL
1	A	60	THR
1	A	62	THR
1	A	63	GLN
1	A	65	ILE
1	A	67	GLN
1	A	76	MET
1	A	82	SER
1	A	84	SER
1	A	89	GLN
1	A	90	ILE
1	A	137	LEU
1	A	145	THR
1	A	164	ASP
1	A	166	ILE
1	A	175	VAL
1	A	225	VAL
1	A	235	ILE
1	A	244	GLU
1	A	254	ASN
1	A	255	GLN
1	A	302	THR
1	A	310	LEU
1	A	321	LEU
1	A	322	LYS
1	A	330	THR
1	A	335	ILE
1	A	336	SER
1	A	337	ILE
1	A	341	VAL
1	A	344	LEU
1	A	356	TYR
1	A	357	LEU
1	A	365	THR
1	A	370	ILE
1	A	376	LEU
1	A	382	VAL
1	A	394	THR
1	A	400	LEU
1	A	406	VAL
1	A	416	VAL
1	A	417	GLU

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Mol	Chain	Res	Type
1	A	419	VAL
1	A	422	GLU
1	A	428	LYS
1	A	435	MET
1	A	443	VAL
1	A	445	ILE
1	A	447	MET
1	A	448	VAL
1	A	452	VAL
1	A	473	THR
1	A	475	VAL
1	A	480	LEU
1	A	489	THR
1	A	492	LEU
1	A	498	LYS
1	A	519	MET
1	A	528	THR
1	A	536	ARG
1	A	547	ILE
1	A	548	ILE
1	A	549	VAL
1	A	552	MET
1	A	571	VAL
1	A	576	VAL
1	A	577	GLN
1	A	578	LEU
1	A	583	THR
1	A	588	GLN
1	A	595	THR
1	A	597	TYR
1	A	603	LYS
1	A	613	ASN
1	A	620	ARG
1	A	626	ILE
1	A	629	VAL
1	A	630	SER
1	A	634	TRP
1	A	636	ASP
1	A	645	GLU
1	A	659	LYS
1	A	666	PHE
1	A	667	ASN

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Mol	Chain	Res	Type
1	A	668	LEU
1	A	671	ILE
1	A	673	GLU
1	A	674	LEU
1	A	678	THR
1	A	687	GLN
1	A	701	GLN
1	A	711	ASP
1	A	713	LEU
1	A	714	THR
1	A	717	ARG
1	A	724	THR
1	A	739	LEU
1	A	745	ASP
1	A	773	VAL
1	A	775	SER
1	A	776	GLU
1	A	780	ARG
1	A	788	ASP
1	A	810	GLU
1	A	815	ARG
1	A	820	ASN
1	A	827	ILE
1	A	828	LEU
1	A	837	THR
1	A	843	LEU
1	A	855	VAL
1	A	868	LEU
1	A	876	LEU
1	A	881	LEU
1	A	887	CYS
1	A	888	LEU
1	A	895	TRP
1	A	902	MET
1	A	904	VAL
1	A	910	ILE
1	A	923	ASN
1	A	935	ILE
1	A	945	ILE
1	A	948	PHE
1	A	954	ASP
1	A	960	LEU

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Mol	Chain	Res	Type
1	A	962	GLU
1	A	968	VAL
1	A	971	ARG
1	A	972	LEU
1	A	983	ILE
1	A	986	VAL
1	A	993	THR
1	A	997	SER
1	A	1005	THR
1	A	1007	VAL
1	A	1011	MET
1	A	1017	LEU
1	A	1019	ILE
1	B	13	TRP
1	B	19	ILE
1	B	21	LEU
1	B	27	ILE
1	B	29	LYS
1	B	30	LEU
1	B	34	GLN
1	B	37	THR
1	B	56	THR
1	B	60	THR
1	B	65	ILE
1	B	69	MET
1	B	70	ASN
1	B	85	THR
1	B	96	SER
1	B	104	GLN
1	B	105	VAL
1	B	121	GLU
1	B	125	GLN
1	B	131	LYS
1	B	136	PHE
1	B	137	LEU
1	B	143	ILE
1	B	145	THR
1	B	150	THR
1	B	151	GLN
1	B	155	SER
1	B	156	ASP
1	B	164	ASP

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Mol	Chain	Res	Type
1	B	176	GLN
1	B	185	ARG
1	B	188	MET
1	B	204	ILE
1	B	213	GLN
1	B	222	THR
1	B	226	LYS
1	B	231	ASN
1	B	235	ILE
1	B	238	THR
1	B	241	THR
1	B	251	LEU
1	B	254	ASN
1	B	256	ASP
1	B	261	LEU
1	B	262	LEU
1	B	289	LEU
1	B	292	LYS
1	B	293	LEU
1	B	295	THR
1	B	300	LEU
1	B	302	THR
1	B	330	THR
1	B	341	VAL
1	B	343	THR
1	B	346	GLU
1	B	349	ILE
1	B	350	LEU
1	B	351	VAL
1	B	372	VAL
1	B	389	SER
1	B	402	ILE
1	B	417	GLU
1	B	420	MET
1	B	429	GLU
1	B	435	MET
1	B	438	ILE
1	B	452	VAL
1	B	456	MET
1	B	468	ARG
1	B	469	GLN
1	B	480	LEU

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Mol	Chain	Res	Type
1	B	482	VAL
1	B	483	LEU
1	B	488	LEU
1	B	497	LEU
1	B	519	MET
1	B	530	SER
1	B	544	LEU
1	B	546	LEU
1	B	547	ILE
1	B	550	VAL
1	B	554	TYR
1	B	562	SER
1	B	571	VAL
1	B	599	LEU
1	B	603	LYS
1	B	605	ASN
1	B	606	VAL
1	B	607	GLU
1	B	620	ARG
1	B	623	ASN
1	B	624	THR
1	B	626	ILE
1	B	629	VAL
1	B	642	ASN
1	B	643	LYS
1	B	644	VAL
1	B	653	ARG
1	B	658	ILE
1	B	659	LYS
1	B	660	ASP
1	B	668	LEU
1	B	681	ASP
1	B	684	LEU
1	B	695	LEU
1	B	702	LEU
1	B	712	MET
1	B	714	THR
1	B	717	ARG
1	B	726	GLN
1	B	741	VAL
1	B	750	LEU
1	B	770	LYS

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Mol	Chain	Res	Type
1	B	776	GLU
1	B	778	LYS
1	B	779	TYR
1	B	799	VAL
1	B	801	PHE
1	B	808	ARG
1	B	817	GLU
1	B	818	ARG
1	B	825	MET
1	B	843	LEU
1	B	867	ARG
1	B	871	ASN
1	B	876	LEU
1	B	879	ILE
1	B	891	LEU
1	B	893	GLU
1	B	897	ILE
1	B	900	SER
1	B	910	ILE
1	B	919	ARG
1	B	922	THR
1	B	925	VAL
1	B	945	ILE
1	B	948	PHE
1	B	952	LEU
1	B	958	LYS
1	B	966	ASP
1	B	972	LEU
1	B	973	ARG
1	B	978	THR
1	B	991	ILE
1	B	993	THR
1	B	1007	VAL
1	B	1022	VAL
1	C	6	ILE
1	C	10	ILE
1	C	13	TRP
1	C	34	GLN
1	C	35	TYR
1	C	38	ILE
1	C	44	THR
1	C	46	SER

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Mol	Chain	Res	Type
1	C	48	SER
1	C	60	THR
1	C	63	GLN
1	C	69	MET
1	C	75	LEU
1	C	84	SER
1	C	91	THR
1	C	108	GLN
1	C	111	LEU
1	C	118	LEU
1	C	123	GLN
1	C	128	SER
1	C	131	LYS
1	C	134	SER
1	C	135	SER
1	C	137	LEU
1	C	152	GLU
1	C	155	SER
1	C	158	VAL
1	C	177	LEU
1	C	186	ILE
1	C	189	ASN
1	C	192	GLU
1	C	204	ILE
1	C	205	THR
1	C	208	LYS
1	C	222	THR
1	C	226	LYS
1	C	230	LEU
1	C	233	SER
1	C	238	THR
1	C	240	LEU
1	C	244	GLU
1	C	249	ILE
1	C	255	GLN
1	C	263	ARG
1	C	269	GLU
1	C	274	ASN
1	C	284	GLN
1	C	295	THR
1	C	302	THR
1	C	307	ARG

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Mol	Chain	Res	Type
1	C	330	THR
1	C	344	LEU
1	C	348	ILE
1	C	355	MET
1	C	369	THR
1	C	372	VAL
1	C	377	LEU
1	C	386	PHE
1	C	394	THR
1	C	398	MET
1	C	406	VAL
1	C	410	ILE
1	C	417	GLU
1	C	422	GLU
1	C	438	ILE
1	C	454	VAL
1	C	456	MET
1	C	459	PHE
1	C	463	THR
1	C	475	VAL
1	C	483	LEU
1	C	496	MET
1	C	497	LEU
1	C	515	TRP
1	C	520	PHE
1	C	543	VAL
1	C	544	LEU
1	C	555	LEU
1	C	564	LEU
1	C	571	VAL
1	C	575	MET
1	C	578	LEU
1	C	588	GLN
1	C	591	LEU
1	C	596	HIS
1	C	624	THR
1	C	652	THR
1	C	658	ILE
1	C	659	LYS
1	C	662	MET
1	C	671	ILE
1	C	678	THR

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Mol	Chain	Res	Type
1	C	685	ILE
1	C	686	ASP
1	C	687	GLN
1	C	693	GLU
1	C	695	LEU
1	C	696	THR
1	C	699	ARG
1	C	713	LEU
1	C	717	ARG
1	C	724	THR
1	C	726	GLN
1	C	731	ILE
1	C	741	VAL
1	C	750	LEU
1	C	767	ARG
1	C	771	VAL
1	C	773	VAL
1	C	791	VAL
1	C	799	VAL
1	C	808	ARG
1	C	815	ARG
1	C	851	LEU
1	C	868	LEU
1	C	872	GLN
1	C	876	LEU
1	C	884	VAL
1	C	901	VAL
1	C	903	LEU
1	C	910	ILE
1	C	921	LEU
1	C	941	ASN
1	C	982	PHE
1	C	984	LEU
1	C	989	LEU
1	C	993	THR
1	C	1028	VAL
1	C	1035	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN

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Mol	Chain	Res	Type
1	A	89	GLN
1	A	106	GLN
1	A	108	GLN
1	A	109	ASN
1	A	125	GLN
1	A	191	ASN
1	A	197	GLN
1	A	210	GLN
1	A	229	GLN
1	A	254	ASN
1	A	282	ASN
1	A	361	ASN
1	A	415	ASN
1	A	437	GLN
1	A	577	GLN
1	A	588	GLN
1	A	592	ASN
1	A	613	ASN
1	A	622	GLN
1	A	667	ASN
1	A	687	GLN
1	A	692	HIS
1	A	701	GLN
1	A	709	HIS
1	A	719	ASN
1	A	733	GLN
1	A	846	GLN
1	A	872	GLN
1	A	923	ASN
1	B	3	ASN
1	B	58	GLN
1	B	67	GLN
1	B	89	GLN
1	B	106	GLN
1	B	108	GLN
1	B	109	ASN
1	B	112	GLN
1	B	124	GLN
1	B	125	GLN
1	B	144	ASN
1	B	161	ASN
1	B	189	ASN

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Mol	Chain	Res	Type
1	B	210	GLN
1	B	213	GLN
1	B	231	ASN
1	B	274	ASN
1	B	526	HIS
1	B	605	ASN
1	B	613	ASN
1	B	622	GLN
1	B	700	ASN
1	B	726	GLN
1	B	744	ASN
1	B	846	GLN
1	B	865	GLN
1	C	3	ASN
1	C	34	GLN
1	C	58	GLN
1	C	63	GLN
1	C	68	ASN
1	C	74	ASN
1	C	104	GLN
1	C	144	ASN
1	C	151	GLN
1	C	176	GLN
1	C	189	ASN
1	C	191	ASN
1	C	197	GLN
1	C	210	GLN
1	C	213	GLN
1	C	231	ASN
1	C	237	GLN
1	C	255	GLN
1	C	274	ASN
1	C	284	GLN
1	C	360	GLN
1	C	361	ASN
1	C	588	GLN
1	C	604	ASN
1	C	605	ASN
1	C	642	ASN
1	C	700	ASN
1	C	726	GLN
1	C	820	ASN

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Mol	Chain	Res	Type
1	C	846	GLN
1	C	865	GLN
1	C	872	GLN
1	C	923	ASN
1	C	941	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	RFP	C	2002	-	63,63,63	2.10	3 (4%)	94,94,94	1.77	16 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RFP	C	2002	-	-	16/60/85/85	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2002	RFP	O4-C11	14.38	1.43	1.21
2	C	2002	RFP	O7-C35	5.67	1.47	1.35
2	C	2002	RFP	O5-C29	3.42	1.48	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2002	RFP	O4-C11-C5	-8.97	115.09	131.63
2	C	2002	RFP	O7-C35-C36	4.63	119.35	111.09
2	C	2002	RFP	O4-C11-C12	-4.13	112.25	120.56
2	C	2002	RFP	O3-C6-C7	4.00	127.95	121.16
2	C	2002	RFP	C41-C42-N4	3.80	116.96	110.86
2	C	2002	RFP	C12-O5-C29	3.75	127.07	117.84
2	C	2002	RFP	C12-C11-C5	-3.24	101.03	107.30
2	C	2002	RFP	C30-C16-C17	-3.01	116.36	123.67
2	C	2002	RFP	C42-N4-C39	2.91	114.17	109.54
2	C	2002	RFP	O7-C25-C26	2.80	113.96	107.52
2	C	2002	RFP	C20-C21-C22	2.75	120.56	114.97
2	C	2002	RFP	C3-C43-N2	2.48	125.64	121.58
2	C	2002	RFP	C42-C41-N3	2.36	114.34	110.51
2	C	2002	RFP	C40-C39-N4	2.11	114.25	110.86
2	C	2002	RFP	C17-C18-C19	-2.03	119.72	124.43
2	C	2002	RFP	C32-C22-C21	2.01	115.38	111.43

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2002	RFP	C2-C3-C43-N2
2	C	2002	RFP	C4-C3-C43-N2
2	C	2002	RFP	C26-C27-O6-C37
2	C	2002	RFP	C28-C27-O6-C37
2	C	2002	RFP	C43-N2-N3-C40
2	C	2002	RFP	C36-C35-O7-C25
2	C	2002	RFP	O8-C35-O7-C25
2	C	2002	RFP	C32-C22-C23-O9
2	C	2002	RFP	C32-C22-C23-C24

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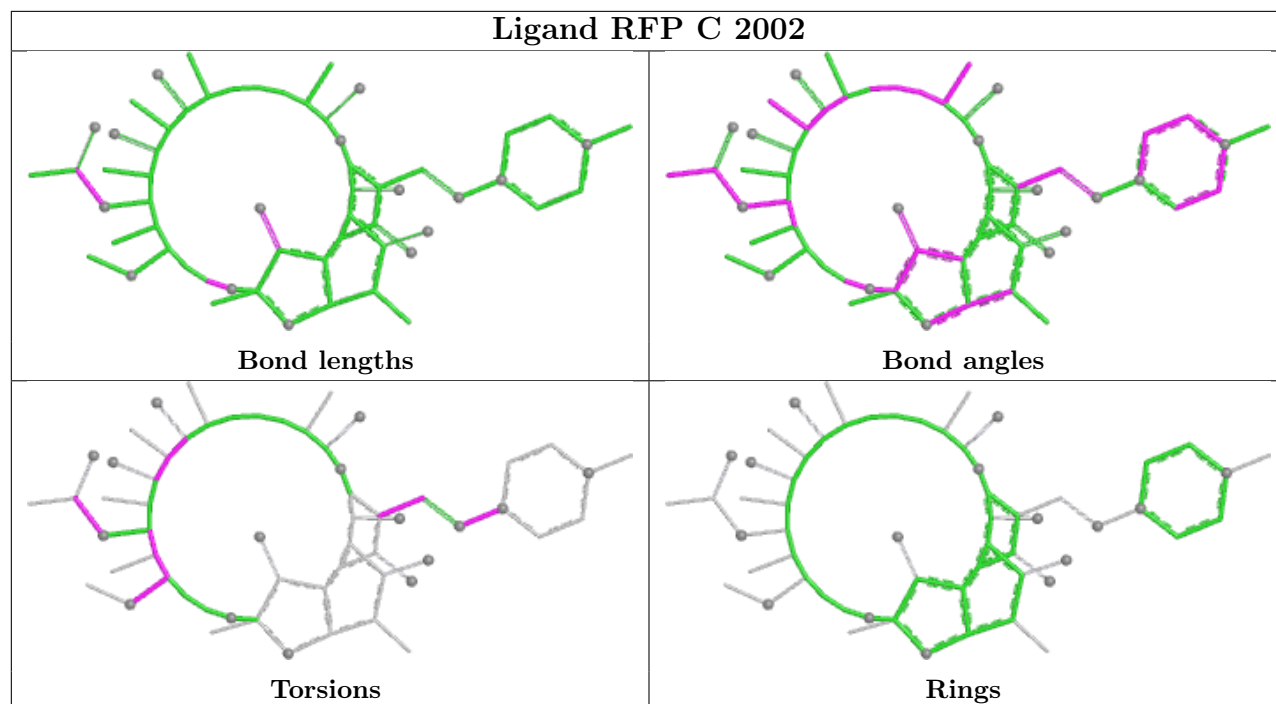
Mol	Chain	Res	Type	Atoms
2	C	2002	RFP	C21-C22-C23-C24
2	C	2002	RFP	C21-C22-C23-O9
2	C	2002	RFP	O10-C21-C22-C32
2	C	2002	RFP	O7-C25-C26-C27
2	C	2002	RFP	O7-C25-C26-C34
2	C	2002	RFP	C34-C26-C27-O6
2	C	2002	RFP	C25-C26-C27-O6

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2002	RFP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	1022/1053 (97%)	0.18	24 (2%) 61 45	40, 90, 124, 144	0
1	B	1022/1053 (97%)	0.30	23 (2%) 61 45	57, 97, 133, 162	0
1	C	1022/1053 (97%)	0.21	25 (2%) 59 44	35, 89, 138, 167	0
All	All	3066/3159 (97%)	0.23	72 (2%) 61 45	35, 92, 134, 167	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	920	GLY	5.5
1	B	991	ILE	4.2
1	C	671	ILE	4.1
1	B	960	LEU	4.0
1	A	989	LEU	3.8
1	A	443	VAL	3.8
1	A	566	ASP	3.7
1	C	960	LEU	3.7
1	C	921	LEU	3.6
1	A	32	VAL	3.5
1	B	902	MET	3.4
1	B	993	THR	3.2
1	A	572	PHE	3.2
1	A	967	ALA	3.1
1	B	527	TYR	3.0
1	A	960	LEU	2.9
1	C	944	LEU	2.9
1	B	438	ILE	2.9
1	B	958	LYS	2.9
1	C	945	ILE	2.9
1	B	563	PHE	2.8
1	C	670	ALA	2.8
1	A	645	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	674	LEU	2.8
1	C	425	LEU	2.6
1	B	672	VAL	2.6
1	B	7	ASP	2.5
1	A	491	ALA	2.5
1	A	676	THR	2.5
1	B	524	THR	2.5
1	B	516	PHE	2.4
1	C	7	ASP	2.4
1	B	673	GLU	2.4
1	C	965	LEU	2.4
1	B	851	LEU	2.4
1	B	832	ALA	2.4
1	A	918	PHE	2.4
1	B	992	SER	2.4
1	A	582	ALA	2.3
1	C	669	PRO	2.3
1	A	222	THR	2.3
1	A	916	ALA	2.3
1	A	772	TYR	2.3
1	A	660	ASP	2.3
1	B	355	MET	2.3
1	B	989	LEU	2.3
1	A	811	TYR	2.3
1	C	964	THR	2.2
1	A	872	GLN	2.2
1	A	995	ALA	2.2
1	A	221	GLY	2.2
1	C	535	LEU	2.2
1	C	870	GLY	2.2
1	A	870	GLY	2.2
1	C	931	LEU	2.1
1	C	665	ALA	2.1
1	B	604	ASN	2.1
1	C	623	ASN	2.1
1	C	664	PHE	2.1
1	B	421	ALA	2.1
1	C	712	MET	2.1
1	C	9	PRO	2.1
1	A	945	ILE	2.0
1	B	357	LEU	2.0
1	B	1017	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	532	GLY	2.0
1	C	905	VAL	2.0
1	C	674	LEU	2.0
1	C	619	GLY	2.0
1	A	360	GLN	2.0
1	A	558	ARG	2.0
1	C	658	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

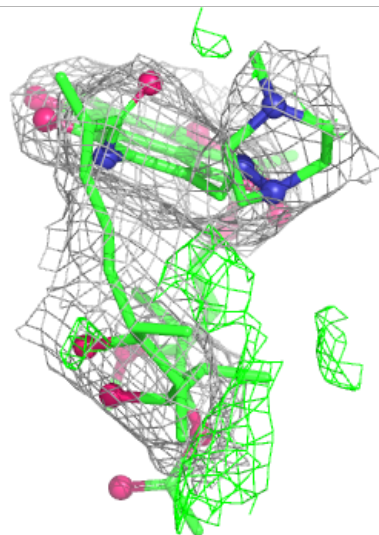
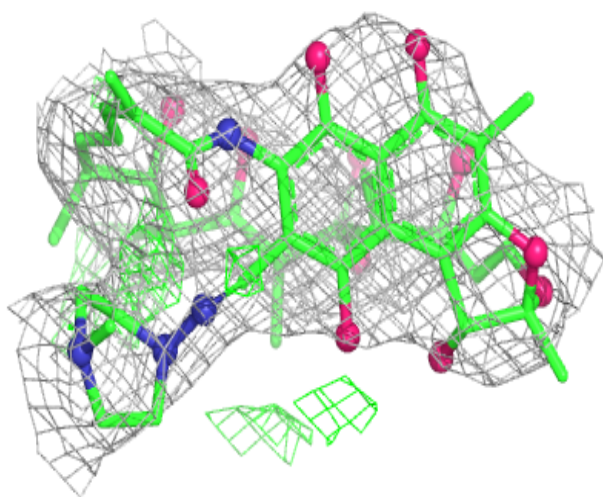
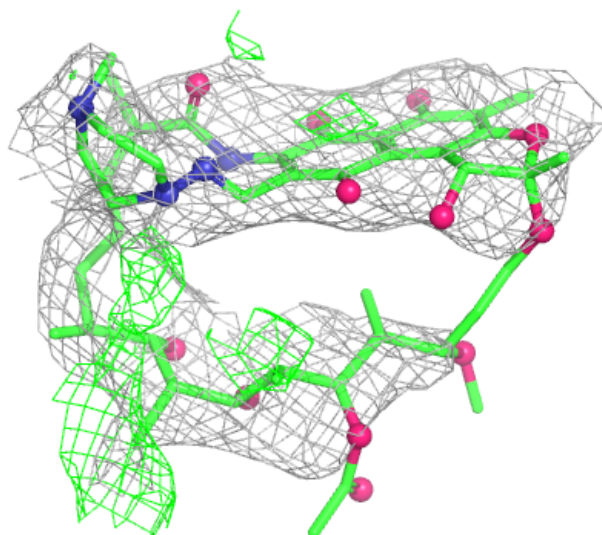
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RFP	C	2002	59/59	0.85	0.22	100,104,105,105	59

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around RFP C 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.