



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AOC
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 : 3.34 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

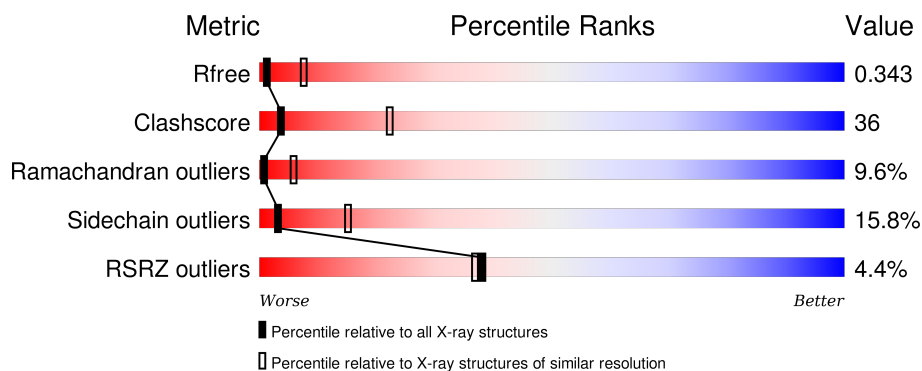
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

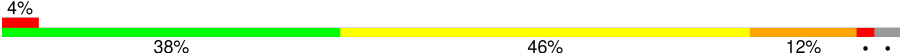
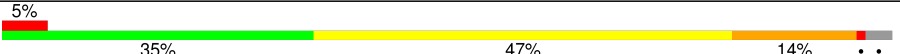
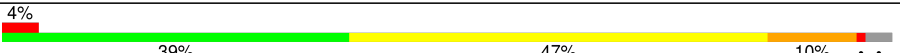
The reported resolution of this entry is 3.34 Å.

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}	91344	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 4% 38% 46% 12% . .
1	B	1053	 5% 35% 47% 14% . .
1	C	1053	 4% 39% 47% 10% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23378 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.

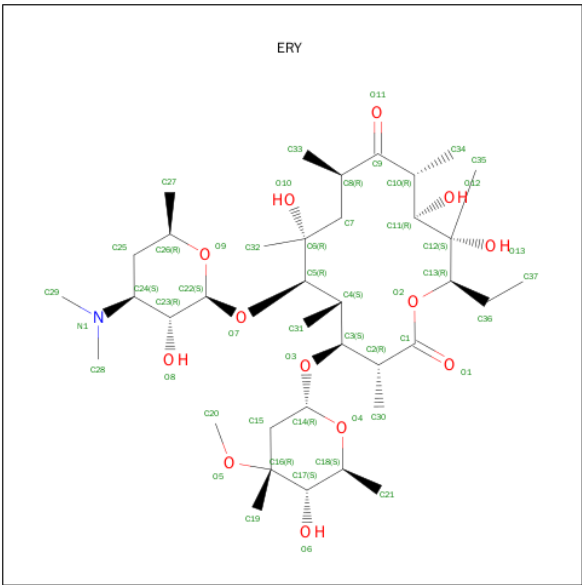
- Molecule 1 is a protein called Acriflavine resistance protein B.

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 ERYTHROMYCIN A (three-letter code: ERY) (formula: C₃₇H₆₇NO₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			51	37	1	13		

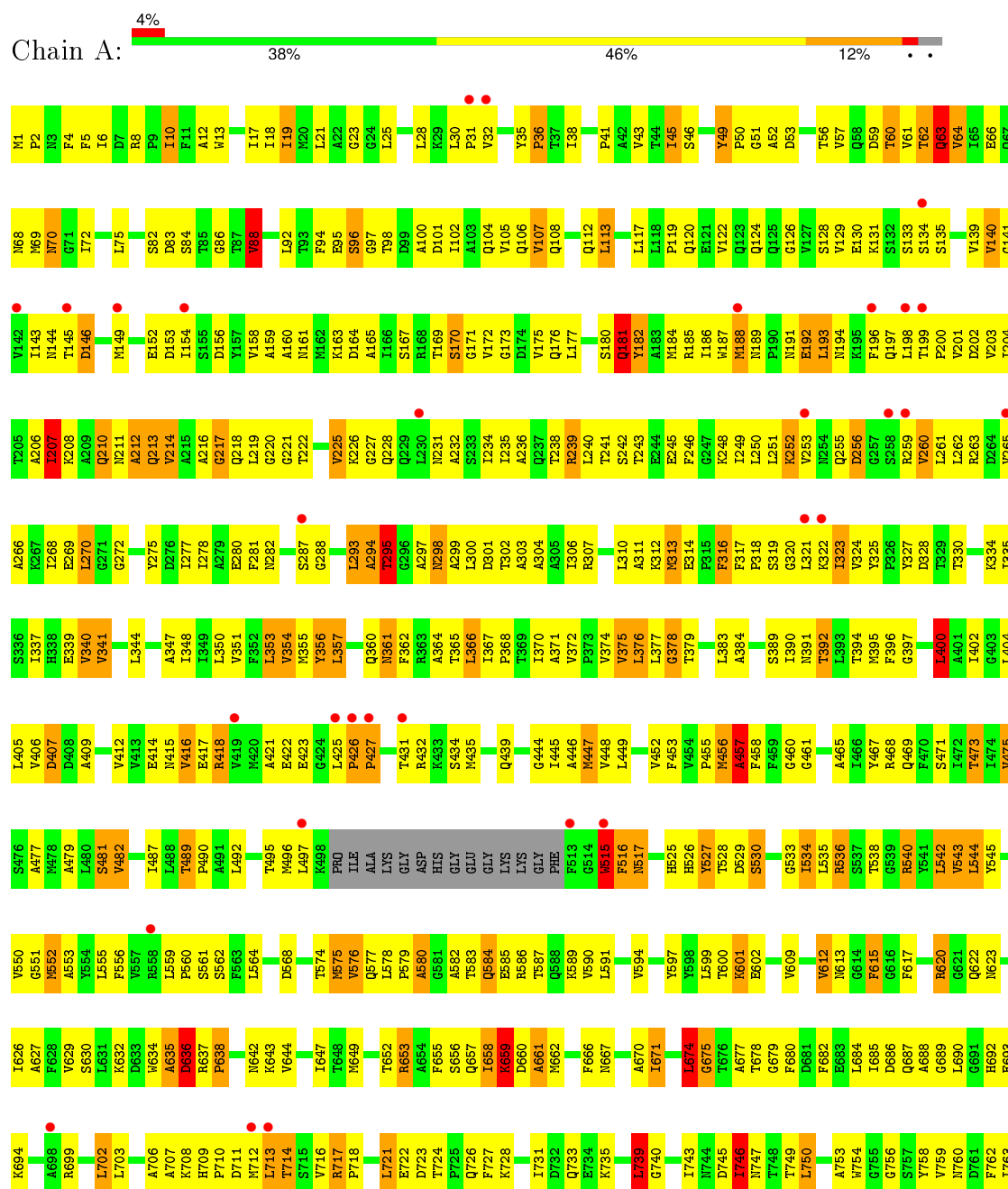
- Molecule 3 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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



G1009	L876	R941	L578	R650	E722	G796	L876	R941	G1009
G1010	L877	A942	P579	R653	D723	Q797	L877	A942	G1010
M1011	A878	L943	R586	A654	T724	M798	A878	L943	M1011
A1014	L879	L944	T587	F655	P725	V799	L879	L944	A1014
T1015	S880	L945	Q588	S656	P800	F801	S880	L945	T1015
V1016	L881	V946	V589	Q657	F727	S802	L881	V946	V1016
L1017	L882	E947	V590	L658	I731	F803	L882	E947	L1017
A1018	V883	F948	L591	A661	D732	A803	V883	F948	A1018
I1019	V884	A949	N592	E662	F733	F804	V884	A949	I1019
F1020	L885	K950	E593	E734	Q733	S805	L885	K950	F1020
F1021	L886	D951	V594	E736	E734	S806	L886	D951	F1021
V1022	C887	L952	T595	A736	K735	S807	C887	L952	V1022
P1023	L888	N953	H596	Q737	A736	R808	L888	N953	P1023
V1024	A889	D954	H597	A738	Q737	W809	A889	D954	V1024
F1025	E893	G957	Y598	L688	L739	G812	E893	G957	F1025
V1028	S894	K958	Y599	L671	G740	R815	S894	K958	V1028
V1029	W895	G959	L599	V672	V741	R819	W895	G959	V1029
R1030	S896	L660	T600	E673	S742	Y819	S896	L660	R1030
R1031	E962	E961	K601	E674	I743	N820	E962	E961	R1031
R1032	A963	A963	K602	E675	I746	N820	A963	A963	R1032
F1033	T964	T964	K603	T676	I746	N820	T964	T964	F1033
S1034	L965	L965	N604	G679	L750	S824	S1034	L965	S1034
R1035	V968	V968	N605	G679	L750	M825	R1035	V968	R1035
K1036	R969	R969	V606	G679	L750	M825	K1036	R969	K1036
ASN	G970	G970	V607	G680	A752	Q830	ASN	G970	ASN
GLU	R971	R971	S608	D681	A752	A831	GLU	R971	GLU
ASP	L972	L972	V610	E682	A754	A831	ASP	L972	ASP
ILE	R973	R973	A611	E683	W754	A832	ILE	R973	ILE
GLU	P974	P974	A612	E684	I758	P833	GLU	P974	GLU
HIS	L975	L975	N613	D686	V759	P833	HIS	L975	HIS
SER	G976	G976	G614	Q687	W760	G834	SER	G976	SER
HIS	N977	N977	G615	A688	D761	K835	HIS	N977	HIS
THR	T978	T978	G616	G689	F762	T837	THR	T978	THR
VAL	S979	S979	F617	L690	I763	G838	VAL	S979	VAL
ASP	F982	F982	A618	G691	R767	E839	ASP	F982	ASP
HIS	L983	L983	G619	H692	W768	A840	HIS	L983	HIS
HIS	L984	L984	R620	E693	V768	M841	HIS	L984	HIS
HIS	G985	G985	T624	E694	K769	E842	HIS	G985	HIS
HIS	V986	V986	F628	L695	K770	L843	HIS	V986	HIS
HIS	N987	N987	V629	T696	V771	Q846	HIS	N987	HIS
HIS	P988	P988	S630	R699	M774	L847	HIS	P988	HIS
HIS	V990	V990	L631	L702	S775	L851	HIS	V990	HIS
HIS	T993	T993	D632	E705	K778	P852	HIS	T993	HIS
HIS	S997	S997	W634	K708	Y779	W859	HIS	S997	HIS
HIS	A999	A999	A635	H709	W781	T860	HIS	A999	HIS
G1004	V1003	V1003	D636	M712	L782	G861	G1004	V1003	G1004
T1005	G1004	G1004	R637	L713	P783	M862	T1005	G1004	T1005
G1006	T1005	T1005	E641	T714	I786	Q865	G1006	T1005	G1006
V1007	G1006	G1006	N642	S715	W789	E866	V1007	G1006	V1007
M1008	A939	A939	K643	V716	Y790	R867	M1008	A939	M1008
	N871	N871	A646	N719	V791	L868		N871	
	Q872	Q872	T647	G720	R792			Q872	
			M649	L721	D795				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.28Å 134.21Å 162.05Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	45.73 – 3.34 45.73 – 3.34	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.73-3.34) 95.4 (45.73-3.34)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.91 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.273 , 0.344 0.269 , 0.343	Depositor DCC
R_{free} test set	3329 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	97.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 74.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	1 of 66210 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23378	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ERY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/7920	0.77	6/10756 (0.1%)
1	B	0.59	0/7920	0.75	4/10756 (0.0%)
1	C	0.63	0/7920	0.78	6/10756 (0.1%)
All	All	0.61	0/23760	0.77	16/32268 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	ALA	N-CA-CB	-19.94	82.18	110.10
1	A	456	MET	N-CA-C	7.14	130.27	111.00
1	C	960	LEU	CA-CB-CG	6.55	130.38	115.30
1	B	960	LEU	CA-CB-CG	6.32	129.83	115.30
1	C	578	LEU	CA-CB-CG	6.10	129.34	115.30
1	C	137	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	400	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	674	LEU	CA-CB-CG	5.73	128.48	115.30
1	C	673	GLU	N-CA-C	-5.64	95.76	111.00
1	A	739	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	193	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	88	VAL	CB-CA-C	-5.17	101.57	111.40
1	B	118	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	674	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	111	LEU	CA-CB-CG	5.10	127.02	115.30
1	B	230	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

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	510	0
1	B	7774	0	7931	626	0
1	C	7774	0	7931	611	0
2	C	51	0	67	10	0
3	A	2	0	0	1	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	23378	0	23860	1686	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 36.

All (1686) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.24	1.16
1:A:145:THR:HG22	1:A:320:GLY:HA3	1.15	1.13
1:A:710:PRO:HA	1:A:713:LEU:HD22	1.19	1.12
1:A:638:PRO:HD2	1:A:642:ASN:HD22	1.04	1.07
1:A:714:THR:HG23	1:A:832:ALA:HA	1.33	1.06
1:A:317:PHE:HB3	1:A:321:LEU:HB2	1.36	1.05
1:A:414:GLU:HG2	1:A:974:PRO:HG3	1.35	1.05
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.41	1.02
1:A:94:PHE:HB3	1:A:98:THR:HG21	1.39	1.02
1:A:674:LEU:HD22	1:A:675:GLY:H	1.25	1.01
1:A:945:ILE:HG13	1:A:971:ARG:HG2	1.40	1.01
1:C:577:GLN:HB3	1:C:624:THR:HG22	1.41	1.01
1:C:415:ASN:HA	1:C:418:ARG:HE	1.23	1.01
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.24	1.00
1:B:879:ILE:O	1:B:883:VAL:HG23	1.58	1.00
1:B:52:ALA:HB2	1:B:86:GLY:N	1.76	1.00
1:C:34:GLN:HE22	1:C:299:ALA:HB3	1.26	0.99
1:B:445:ILE:HG23	1:B:940:LYS:HG3	1.44	0.99
1:C:930:GLY:HA3	1:C:1007:VAL:HG22	1.43	0.98
1:A:140:VAL:HG12	1:A:141:GLY:H	1.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.44	0.98
1:A:447:MET:HB3	1:A:887:CYS:SG	2.04	0.98
1:C:901:VAL:HG11	1:C:943:ILE:HG13	1.43	0.97
1:C:26:ALA:O	1:C:30:LEU:HB2	1.63	0.96
1:A:659:LYS:HG2	1:A:660:ASP:H	1.27	0.96
1:C:418:ARG:HH12	1:C:971:ARG:HH11	1.06	0.95
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.46	0.95
1:C:240:LEU:HD12	1:C:245:GLU:HB3	1.48	0.94
1:A:246:PHE:O	1:A:249:ILE:HG12	1.68	0.94
1:A:145:THR:CG2	1:A:320:GLY:HA3	1.97	0.94
1:C:23:GLY:HA3	1:C:377:LEU:O	1.69	0.93
1:A:756:GLY:HA2	1:A:774:MET:HB2	1.52	0.92
1:B:574:THR:HG23	1:B:665:ALA:HB2	1.51	0.92
1:C:713:LEU:HD11	1:C:834:GLY:HA3	1.52	0.91
1:C:959:GLY:H	1:C:962:GLU:HB2	1.36	0.90
1:B:485:ALA:HA	1:B:489:THR:HB	1.54	0.90
1:A:638:PRO:HD2	1:A:642:ASN:ND2	1.87	0.89
1:B:26:ALA:O	1:B:30:LEU:HB2	1.73	0.89
1:A:710:PRO:CA	1:A:713:LEU:HD22	2.03	0.89
1:C:979:SER:O	1:C:983:ILE:HG12	1.72	0.88
1:A:795:ASP:HB2	1:A:797:GLN:HG2	1.54	0.88
1:B:743:ILE:H	1:B:743:ILE:HD12	1.37	0.88
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.55	0.87
1:B:631:LEU:HB3	1:B:637:ARG:HH12	1.39	0.87
1:B:222:THR:OG1	1:B:223:PRO:HD3	1.75	0.87
1:C:404:LEU:HD22	1:C:478:MET:HG3	1.56	0.87
1:C:409:ALA:O	1:C:413:VAL:HG12	1.72	0.87
1:C:972:LEU:H	1:C:974:PRO:HD2	1.39	0.87
1:A:140:VAL:HG12	1:A:141:GLY:N	1.88	0.86
1:B:986:VAL:O	1:B:990:VAL:HG23	1.75	0.86
1:C:11:PHE:O	1:C:14:VAL:HG12	1.76	0.86
1:C:513:PHE:HB2	1:C:516:PHE:HB2	1.58	0.85
1:C:692:HIS:HE1	1:C:721:LEU:HD21	1.38	0.85
1:A:612:VAL:HG23	1:A:626:ILE:HG22	1.58	0.85
1:A:525:HIS:HA	1:A:528:THR:HG22	1.59	0.85
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.56	0.85
1:B:607:GLU:HG2	1:B:632:LYS:HA	1.57	0.84
1:B:583:THR:HG22	1:B:586:ARG:HD3	1.59	0.84
1:A:141:GLY:HA2	1:A:288:GLY:HA2	1.58	0.84
1:B:591:LEU:O	1:B:595:THR:HG22	1.78	0.84
1:A:731:ILE:HD12	1:A:746:ILE:HG21	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASN:HA	1:C:418:ARG:NE	1.93	0.83
1:B:24:GLY:H	1:B:27:ILE:HG23	1.44	0.83
1:C:176:GLN:NE2	1:C:620:ARG:NH1	2.26	0.83
1:C:767:ARG:HH11	1:C:767:ARG:HG3	1.43	0.83
1:C:545:TYR:OH	1:C:1021:PHE:HB3	1.78	0.83
1:B:143:ILE:HD12	1:B:144:ASN:H	1.43	0.82
1:B:736:ALA:HB1	1:B:741:VAL:CG2	2.08	0.82
1:B:193:LEU:HD23	1:B:265:VAL:HG11	1.59	0.82
1:A:13:TRP:O	1:A:17:ILE:HG12	1.77	0.82
1:C:713:LEU:CD1	1:C:834:GLY:HA3	2.09	0.82
1:A:383:LEU:HD21	1:A:473:THR:HG23	1.62	0.82
1:C:343:THR:HG21	1:C:989:LEU:HD13	1.60	0.82
1:B:157:TYR:HA	1:B:161:ASN:ND2	1.95	0.82
1:C:758:TYR:H	1:C:758:TYR:HD1	1.27	0.82
1:C:713:LEU:HD11	1:C:835:LYS:H	1.44	0.82
1:B:401:ALA:HA	1:B:404:LEU:HB2	1.61	0.82
1:C:265:VAL:O	1:C:265:VAL:HG23	1.79	0.81
1:B:235:ILE:N	1:B:235:ILE:HD13	1.96	0.81
1:A:750:LEU:O	1:A:754:TRP:HD1	1.64	0.81
1:A:51:GLY:O	1:C:215:ALA:HB1	1.80	0.80
1:C:416:VAL:HG11	1:C:431:THR:HG22	1.63	0.80
1:B:715:SER:O	1:B:716:VAL:HG23	1.82	0.80
1:A:140:VAL:CG1	1:A:141:GLY:H	1.94	0.80
1:A:591:LEU:CD1	1:A:613:ASN:HB3	2.11	0.80
1:B:563:PHE:HD1	1:B:866:GLU:HG3	1.46	0.80
1:B:359:LEU:HD23	1:B:365:THR:HA	1.62	0.80
1:C:932:LEU:HA	1:C:935:ILE:HG22	1.63	0.79
1:A:6:ILE:HD11	1:A:432:ARG:HD2	1.64	0.79
1:C:400:LEU:HD12	1:C:929:VAL:HG12	1.65	0.79
1:A:883:VAL:O	1:A:887:CYS:HB2	1.82	0.79
1:B:94:PHE:HB3	1:B:98:THR:HG21	1.64	0.79
1:B:673:GLU:O	1:B:676:THR:HG22	1.82	0.79
1:B:143:ILE:HD13	1:B:285:PRO:O	1.83	0.78
1:C:672:VAL:CG1	1:C:673:GLU:H	1.96	0.78
1:C:552:MET:SD	1:C:909:VAL:HG21	2.22	0.78
1:C:983:ILE:HG23	1:C:1008:MET:HG2	1.65	0.78
1:A:396:PHE:CD2	1:A:1003:VAL:HG21	2.18	0.78
1:A:945:ILE:CG1	1:A:971:ARG:HG2	2.13	0.78
1:A:746:ILE:HD12	1:A:791:VAL:HG21	1.64	0.78
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.13	0.78
1:C:712:MET:HA	1:C:835:LYS:HG3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.65	0.78
1:C:605:ASN:HB3	1:C:637:ARG:HD3	1.64	0.78
1:C:144:ASN:ND2	1:C:149:MET:H	1.81	0.77
1:A:552:MET:HE1	1:A:906:PRO:HA	1.65	0.77
1:B:552:MET:SD	1:B:909:VAL:HG21	2.24	0.77
1:C:832:ALA:HB1	1:C:833:PRO:CD	2.15	0.77
1:B:225:VAL:H	1:C:781:MET:HE3	1.49	0.76
1:B:149:MET:HB3	1:B:154:ILE:HG22	1.67	0.76
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.66	0.76
1:B:157:TYR:HA	1:B:161:ASN:HD22	1.48	0.76
1:A:278:ILE:HB	1:A:613:ASN:OD1	1.86	0.76
1:B:224:PRO:HA	1:C:781:MET:HE3	1.68	0.76
1:C:34:GLN:HE22	1:C:299:ALA:CB	1.99	0.76
1:C:894:SER:OG	1:C:897:ILE:HG12	1.86	0.76
1:A:890:ALA:HB1	1:C:11:PHE:HD1	1.50	0.76
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.65	0.76
1:C:588:GLN:HG2	1:C:613:ASN:HD22	1.51	0.76
1:B:343:THR:HG21	1:B:1000:GLN:OE1	1.84	0.76
1:B:399:VAL:O	1:B:402:ILE:HG22	1.85	0.76
1:A:702:LEU:HD21	1:A:844:MET:HE1	1.68	0.75
1:B:213:GLN:HB2	1:B:239:ARG:HD2	1.67	0.75
1:A:404:LEU:HD21	1:A:449:LEU:HD13	1.68	0.75
1:A:43:VAL:HG11	1:A:107:VAL:HG21	1.66	0.75
1:A:396:PHE:HD2	1:A:1003:VAL:HG21	1.51	0.75
1:B:552:MET:SD	1:B:909:VAL:CG2	2.74	0.75
2:C:3402:ERY:H14	2:C:3402:ERY:H302	1.68	0.75
1:A:354:VAL:HG12	1:A:355:MET:H	1.50	0.75
1:A:344:LEU:HD13	1:A:376:LEU:HD21	1.68	0.75
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.21	0.75
1:B:934:THR:C	1:B:936:GLY:H	1.90	0.74
1:B:934:THR:O	1:B:936:GLY:N	2.20	0.74
1:C:448:VAL:HG22	1:C:887:CYS:HB3	1.68	0.74
1:C:618:ALA:HB1	1:C:815:ARG:HH12	1.52	0.74
1:B:923:ASN:HD22	1:B:927:PHE:HD2	1.34	0.74
1:A:445:ILE:HG21	1:A:940:LYS:HG3	1.67	0.74
1:B:924:ASP:O	1:B:928:GLN:HG3	1.87	0.74
1:A:294:ALA:HB3	1:A:297:ALA:HB2	1.70	0.74
1:B:892:TYR:HB3	1:B:897:ILE:HD11	1.68	0.74
1:B:579:PRO:O	1:B:580:ALA:O	2.05	0.74
1:A:659:LYS:HG2	1:A:660:ASP:N	2.03	0.74
1:A:6:ILE:HG22	1:A:490:PRO:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLN:HG3	1:C:56:THR:HG23	1.69	0.74
1:C:176:GLN:HE22	1:C:620:ARG:NH1	1.84	0.73
1:C:375:VAL:HG11	1:C:405:LEU:HD22	1.70	0.73
1:A:707:ALA:HA	1:A:713:LEU:HD12	1.71	0.73
1:B:30:LEU:HD22	1:B:390:ILE:HG13	1.67	0.73
1:C:754:TRP:CZ2	1:C:786:ILE:HD13	2.24	0.73
1:B:242:SER:HB2	1:B:245:GLU:OE2	1.87	0.73
1:B:736:ALA:HB1	1:B:741:VAL:HG23	1.69	0.73
1:A:921:LEU:HG	1:A:922:THR:H	1.51	0.73
1:B:36:PRO:HD3	1:B:391:ASN:ND2	2.04	0.73
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.23	0.73
1:B:203:VAL:O	1:B:207:ILE:HG12	1.88	0.73
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.70	0.73
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.70	0.73
1:A:144:ASN:HD22	1:A:149:MET:H	1.37	0.73
1:B:441:ALA:O	1:B:445:ILE:HG12	1.88	0.73
1:B:213:GLN:CG	1:C:56:THR:HG23	2.18	0.73
1:B:276:ASP:O	1:B:614:GLY:HA3	1.89	0.73
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.71	0.72
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.69	0.72
1:B:426:PRO:HB3	1:B:430:ALA:HB3	1.71	0.72
1:B:119:PRO:HB2	1:B:122:VAL:HG23	1.70	0.72
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.70	0.72
1:B:947:GLU:HA	1:B:947:GLU:OE1	1.88	0.72
1:C:92:LEU:HD12	1:C:92:LEU:H	1.53	0.72
1:A:728:LYS:HD2	1:C:235:ILE:O	1.89	0.72
1:C:681:ASP:HB3	1:C:860:THR:CG2	2.20	0.72
1:C:600:THR:O	1:C:603:LYS:HB2	1.90	0.72
1:A:597:TYR:O	1:A:601:LYS:HB3	1.89	0.72
1:A:188:MET:HA	1:A:266:ALA:HB2	1.72	0.72
1:B:560:PRO:HB2	1:B:836:SER:HB2	1.71	0.72
1:B:675:GLY:O	1:B:677:ALA:N	2.22	0.72
1:C:548:ILE:HD13	1:C:1017:LEU:HD21	1.72	0.71
1:C:203:VAL:O	1:C:207:ILE:HG12	1.90	0.71
1:C:709:HIS:HB3	1:C:712:MET:SD	2.31	0.71
1:A:753:ALA:HB3	1:A:754:TRP:CD1	2.26	0.71
1:C:617:PHE:O	2:C:3402:ERY:H332	1.90	0.71
1:A:170:SER:O	1:A:302:THR:HG22	1.90	0.71
1:C:137:LEU:HD23	1:C:293:LEU:HD13	1.73	0.71
1:A:4:PHE:HB3	1:A:8:ARG:NH2	2.05	0.71
1:C:795:ASP:OD1	1:C:797:GLN:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ILE:HD11	1:C:281:PHE:HB3	1.72	0.70
1:A:207:ILE:HB	1:A:759:VAL:HG11	1.72	0.70
1:C:210:GLN:O	1:C:240:LEU:HD21	1.91	0.70
1:A:10:ILE:HG21	1:B:893:GLU:O	1.90	0.70
1:A:721:LEU:HD12	1:A:814:PRO:HG2	1.73	0.70
1:C:124:GLN:CB	1:C:758:TYR:HE2	2.05	0.70
1:A:782:LEU:O	1:A:785:ASP:HB2	1.91	0.70
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.56	0.70
1:A:471:SER:O	1:A:475:VAL:HG12	1.90	0.70
1:C:418:ARG:NH1	1:C:971:ARG:HH11	1.86	0.69
1:C:166:ILE:HG21	1:C:291:ILE:HD11	1.72	0.69
1:C:713:LEU:HD11	1:C:835:LYS:N	2.06	0.69
1:C:265:VAL:O	1:C:266:ALA:HB2	1.91	0.69
1:A:41:PRO:HB3	1:A:100:ALA:HB2	1.74	0.69
1:B:210:GLN:HG2	1:C:733:GLN:HE21	1.56	0.69
1:A:145:THR:HG21	1:A:322:LYS:HE2	1.73	0.69
1:B:932:LEU:HA	1:B:935:ILE:HG13	1.73	0.69
1:A:714:THR:HG23	1:A:832:ALA:CA	2.19	0.69
1:C:839:GLU:HA	1:C:842:GLU:HB3	1.74	0.69
1:A:591:LEU:HD12	1:A:613:ASN:HB3	1.74	0.69
1:A:314:GLU:HA	1:A:317:PHE:CD2	2.27	0.69
1:C:727:PHE:CE1	1:C:807:SER:HB2	2.28	0.69
1:B:298:ASN:O	1:B:300:LEU:N	2.26	0.69
1:B:66:GLU:OE2	1:B:821:GLY:HA2	1.93	0.69
1:B:460:GLY:HA2	1:B:872:GLN:HE22	1.58	0.69
1:B:897:ILE:HB	1:B:1026:PHE:HE1	1.58	0.69
1:A:707:ALA:HA	1:A:713:LEU:CD1	2.23	0.69
1:A:674:LEU:CD2	1:A:675:GLY:H	2.04	0.69
1:A:746:ILE:HG13	1:A:804:PHE:CE1	2.26	0.69
1:B:344:LEU:O	1:B:348:ILE:HG13	1.93	0.69
1:B:561:SER:O	1:B:838:GLY:HA3	1.93	0.69
1:C:146:ASP:HB3	1:C:148:THR:CG2	2.21	0.68
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.23	0.68
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.75	0.68
1:B:671:ILE:HG22	1:B:676:THR:HB	1.75	0.68
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.29	0.68
1:A:180:SER:O	1:A:181:GLN:HB3	1.91	0.68
1:A:2:PRO:O	1:A:6:ILE:HG23	1.92	0.68
1:B:717:ARG:HH11	1:B:717:ARG:CG	2.06	0.68
1:A:895:TRP:HZ2	1:C:13:TRP:CE3	2.10	0.68
1:B:419:VAL:HG12	1:B:419:VAL:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:GLU:HA	1:C:708:LYS:HE2	1.75	0.68
1:C:607:GLU:HB2	1:C:632:LYS:HG2	1.75	0.68
1:B:775:SER:O	1:B:780:ARG:HD3	1.93	0.68
1:C:435:MET:HA	1:C:438:ILE:HG22	1.75	0.68
1:B:326:PRO:HG2	1:B:610:PHE:CD1	2.28	0.68
1:B:905:VAL:HG13	1:B:906:PRO:HD3	1.76	0.68
1:A:1021:PHE:HD1	1:A:1025:PHE:CE1	2.11	0.68
1:B:68:ASN:C	1:B:70:ASN:H	1.96	0.68
1:B:121:GLU:O	1:B:125:GLN:HG2	1.94	0.68
1:B:880:SER:O	1:B:884:VAL:HG23	1.94	0.68
1:B:18:ILE:HG22	1:B:19:ILE:HD13	1.76	0.68
1:C:973:ARG:O	1:C:977:MET:HB2	1.94	0.68
1:B:456:MET:HG3	1:B:467:TYR:CB	2.13	0.68
1:C:759:VAL:HG23	1:C:771:VAL:O	1.94	0.68
1:C:2:PRO:O	1:C:6:ILE:HG12	1.92	0.68
1:C:672:VAL:HG12	1:C:673:GLU:H	1.59	0.68
1:A:31:PRO:HB2	1:A:389:SER:HB2	1.74	0.68
1:C:734:GLU:HA	1:C:737:GLN:HG2	1.76	0.68
1:A:23:GLY:HA3	1:A:378:GLY:HA2	1.77	0.67
1:A:299:ALA:O	1:A:303:ALA:HB2	1.94	0.67
1:A:844:MET:HA	1:A:844:MET:HE3	1.74	0.67
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.24	0.67
1:A:643:LYS:O	1:A:647:ILE:HG13	1.93	0.67
1:A:207:ILE:O	1:A:211:ASN:HB3	1.94	0.67
1:C:66:GLU:OE2	1:C:80:SER:HB3	1.94	0.67
1:C:767:ARG:HD3	1:C:769:LYS:HE3	1.77	0.67
1:B:717:ARG:HH11	1:B:717:ARG:HG2	1.58	0.67
1:B:411:VAL:HB	1:B:438:ILE:HD11	1.76	0.67
1:C:244:GLU:HA	1:C:263:ARG:NH2	2.05	0.67
1:B:408:ASP:OD1	1:B:442:LEU:HA	1.94	0.67
1:C:681:ASP:CB	1:C:860:THR:HG23	2.24	0.67
1:C:979:SER:O	1:C:983:ILE:CG1	2.41	0.67
1:C:758:TYR:CD1	1:C:758:TYR:N	2.51	0.67
1:C:185:ARG:HB2	1:C:269:GLU:O	1.94	0.67
1:B:94:PHE:CB	1:B:98:THR:HG21	2.24	0.67
1:B:416:VAL:O	1:B:426:PRO:HG2	1.95	0.67
1:B:915:ALA:CB	1:B:1009:GLY:HA3	2.24	0.67
1:B:55:LYS:HE2	1:B:59:ASP:OD1	1.94	0.67
1:C:925:VAL:O	1:C:929:VAL:HG23	1.95	0.67
1:B:582:ALA:O	1:B:583:THR:HB	1.94	0.67
1:B:298:ASN:HB3	1:B:301:ASP:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:CD1	1:A:1003:VAL:HG13	2.24	0.67
1:A:733:GLN:OE1	1:A:743:ILE:HD11	1.95	0.67
1:B:13:TRP:HE3	1:B:488:LEU:HD21	1.60	0.67
1:C:252:LYS:HG2	1:C:260:VAL:HG12	1.76	0.67
1:C:332:PHE:CD2	1:C:569:GLN:HA	2.30	0.67
1:C:3:ASN:C	1:C:5:PHE:H	1.99	0.66
1:A:1:MET:SD	1:A:487:ILE:HD11	2.35	0.66
1:C:542:LEU:HD11	1:C:1028:VAL:HG11	1.76	0.66
1:B:188:MET:HB2	1:B:775:SER:HA	1.76	0.66
1:B:348:ILE:HG12	1:B:402:ILE:HD11	1.75	0.66
1:C:56:THR:O	1:C:60:THR:HB	1.95	0.66
1:C:610:PHE:HB3	1:C:628:PHE:HB2	1.76	0.66
1:C:636:ASP:N	1:C:636:ASP:OD1	2.27	0.66
1:B:149:MET:HB3	1:B:154:ILE:CG2	2.25	0.66
1:C:679:GLY:HA2	1:C:830:GLN:HA	1.76	0.66
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.78	0.66
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.96	0.66
1:A:94:PHE:CB	1:A:98:THR:HG21	2.22	0.66
1:C:616:GLY:HA3	1:C:624:THR:HB	1.76	0.66
1:A:294:ALA:O	1:A:295:THR:HB	1.93	0.66
1:B:419:VAL:O	1:B:426:PRO:HG3	1.95	0.66
1:B:24:GLY:N	1:B:27:ILE:HG23	2.11	0.66
1:A:69:MET:HE1	1:A:107:VAL:HG13	1.77	0.66
1:C:986:VAL:HG12	1:C:986:VAL:O	1.96	0.66
1:B:817:GLU:HB2	1:B:824:SER:O	1.96	0.66
1:B:13:TRP:CE3	1:B:488:LEU:HD21	2.30	0.65
1:B:859:TRP:HB3	1:B:863:SER:HB2	1.78	0.65
1:C:695:LEU:HD22	1:C:825:MET:SD	2.36	0.65
1:C:203:VAL:HG13	1:C:262:LEU:CD1	2.25	0.65
1:C:176:GLN:NE2	1:C:620:ARG:HH11	1.94	0.65
1:C:124:GLN:HB2	1:C:758:TYR:HE2	1.61	0.65
1:A:379:THR:HG21	1:A:477:ALA:HA	1.76	0.65
1:B:249:ILE:HB	1:B:262:LEU:HD12	1.78	0.65
1:B:632:LYS:O	1:B:633:ASP:O	2.15	0.65
1:C:522:LYS:HA	1:C:522:LYS:HE2	1.78	0.65
1:C:641:GLU:O	1:C:650:ARG:NH1	2.30	0.65
1:A:746:ILE:CD1	1:A:791:VAL:HG21	2.27	0.65
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.61	0.65
1:B:911:GLY:HA2	1:B:914:LEU:HB2	1.79	0.65
1:B:952:LEU:C	1:B:954:ASP:H	2.00	0.65
1:C:775:SER:HB3	1:C:780:ARG:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1009:GLY:O	1:B:1012:VAL:HG22	1.97	0.64
1:A:141:GLY:HA2	1:A:288:GLY:CA	2.28	0.64
1:B:925:VAL:HA	1:B:928:GLN:OE1	1.97	0.64
1:A:747:ASN:HD21	1:C:237:GLN:HE21	1.45	0.64
1:B:189:ASN:O	1:B:193:LEU:HB2	1.97	0.64
1:B:213:GLN:HB2	1:B:239:ARG:HG3	1.79	0.64
1:B:157:TYR:CA	1:B:161:ASN:HD22	2.10	0.64
1:A:591:LEU:HD11	1:A:613:ASN:HB3	1.77	0.64
1:B:563:PHE:CD1	1:B:866:GLU:HG3	2.32	0.64
1:B:931:LEU:O	1:B:935:ILE:HG12	1.97	0.64
1:B:144:ASN:HD21	1:B:148:THR:H	1.44	0.64
1:A:171:GLY:HA3	1:A:302:THR:HG21	1.80	0.64
1:B:683:GLU:OE1	1:B:826:GLU:HG3	1.98	0.64
1:A:217:GLY:O	1:A:234:ILE:HG12	1.97	0.64
1:A:714:THR:CG2	1:A:832:ALA:HA	2.19	0.64
1:B:5:PHE:HB3	1:B:12:ALA:HB2	1.80	0.64
1:C:752:ALA:O	1:C:774:MET:HA	1.98	0.64
1:C:688:ALA:O	1:C:690:LEU:N	2.31	0.64
1:A:159:ALA:HA	1:A:163:LYS:HB2	1.79	0.64
1:C:664:PHE:HD2	1:C:664:PHE:H	1.46	0.64
1:C:3:ASN:HD21	1:C:432:ARG:HG3	1.62	0.64
1:C:265:VAL:O	1:C:266:ALA:CB	2.46	0.64
1:B:356:TYR:CE2	1:B:365:THR:HG21	2.33	0.64
1:C:61:VAL:O	1:C:64:VAL:HG23	1.98	0.64
1:A:188:MET:HA	1:A:266:ALA:CB	2.27	0.64
1:C:713:LEU:HD11	1:C:834:GLY:CA	2.26	0.63
1:B:339:GLU:O	1:B:342:LYS:HB3	1.98	0.63
1:A:277:ILE:HD11	1:A:615:PHE:HB3	1.80	0.63
1:A:102:ILE:HD11	1:C:101:ASP:HB3	1.80	0.63
1:C:20:MET:HG3	1:C:374:VAL:HG23	1.80	0.63
1:B:143:ILE:HD12	1:B:144:ASN:N	2.10	0.63
1:B:251:LEU:HD22	1:B:262:LEU:H	1.62	0.63
1:A:117:LEU:HD21	1:C:124:GLN:O	1.98	0.63
1:B:135:SER:HB2	1:B:676:THR:HG21	1.80	0.63
1:A:895:TRP:HZ2	1:C:13:TRP:HE3	1.46	0.63
1:A:886:LEU:CD1	1:C:14:VAL:HG23	2.28	0.63
1:B:762:PHE:HD2	1:B:771:VAL:HG22	1.64	0.63
1:A:530:SER:O	1:A:534:ILE:HG13	1.97	0.63
1:A:731:ILE:HD12	1:A:746:ILE:CG2	2.27	0.63
1:C:144:ASN:HD22	1:C:149:MET:H	1.43	0.63
1:C:897:ILE:N	1:C:898:PRO:HD2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:O	1:A:158:VAL:HG23	1.99	0.63
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.80	0.63
1:A:113:LEU:HG	1:C:127:VAL:HG23	1.81	0.63
1:A:901:VAL:O	1:A:904:VAL:HG23	1.98	0.63
1:C:455:PRO:O	1:C:876:LEU:HD11	1.98	0.63
1:A:620:ARG:HH11	1:A:620:ARG:CG	2.11	0.63
1:A:713:LEU:HD23	1:A:714:THR:H	1.63	0.62
1:B:359:LEU:CD2	1:B:365:THR:HA	2.29	0.62
1:B:111:LEU:HD22	1:B:129:VAL:CG2	2.29	0.62
1:A:890:ALA:HB1	1:C:11:PHE:CD1	2.32	0.62
1:A:145:THR:HG23	1:A:146:ASP:H	1.65	0.62
1:C:246:PHE:O	1:C:249:ILE:HG12	2.00	0.62
1:C:767:ARG:HH11	1:C:767:ARG:CG	2.11	0.62
1:B:349:ILE:C	1:B:351:VAL:H	2.03	0.62
1:B:326:PRO:O	1:B:630:SER:HB2	2.00	0.62
1:B:158:VAL:HA	1:B:162:MET:CG	2.28	0.62
1:B:225:VAL:N	1:C:781:MET:HE3	2.15	0.62
1:A:330:THR:HG22	1:A:334:LYS:HE2	1.82	0.62
1:A:182:TYR:HB3	1:A:270:LEU:HD11	1.82	0.62
1:A:144:ASN:HA	1:A:320:GLY:O	1.99	0.62
1:B:904:VAL:HG13	1:B:907:LEU:HD12	1.82	0.62
1:C:911:GLY:C	1:C:1010:GLY:HA2	2.20	0.62
1:A:717:ARG:HB2	1:A:718:PRO:HD2	1.82	0.62
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.99	0.62
1:C:211:ASN:HD22	1:C:240:LEU:HD23	1.65	0.62
1:B:346:GLU:O	1:B:988:PRO:HG3	2.00	0.62
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.82	0.62
1:B:445:ILE:HD13	1:B:943:ILE:HG23	1.83	0.61
1:A:241:THR:HG22	1:A:763:ILE:O	2.00	0.61
1:A:144:ASN:ND2	1:A:149:MET:H	1.97	0.61
1:A:888:LEU:HD21	1:A:901:VAL:HB	1.82	0.61
1:A:552:MET:CE	1:A:906:PRO:HA	2.29	0.61
1:C:372:VAL:HG21	1:C:406:VAL:HG22	1.82	0.61
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.82	0.61
1:A:713:LEU:HD23	1:A:714:THR:N	2.14	0.61
1:B:680:PHE:O	1:B:828:LEU:HD23	2.00	0.61
1:C:423:GLU:HB3	1:C:426:PRO:HD2	1.81	0.61
1:C:712:MET:SD	1:C:843:LEU:HD22	2.41	0.61
1:B:792:ARG:HG2	1:B:793:ALA:N	2.16	0.61
1:B:714:THR:HG22	1:B:831:ALA:HA	1.82	0.61
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:ASP:HB2	1:C:643:LYS:HG3	1.83	0.61
1:C:16:ALA:HB1	1:C:374:VAL:HG21	1.83	0.61
1:B:859:TRP:HB3	1:B:863:SER:CB	2.30	0.61
1:B:525:HIS:HA	1:B:528:THR:HG22	1.82	0.61
1:B:485:ALA:HA	1:B:489:THR:CB	2.29	0.61
1:A:339:GLU:O	1:A:341:VAL:N	2.33	0.61
1:A:568:ASP:O	1:A:634:TRP:CH2	2.54	0.61
1:B:57:VAL:O	1:B:61:VAL:HG12	2.01	0.61
1:C:142:VAL:HG12	1:C:154:ILE:HG23	1.83	0.61
2:C:3402:ERY:H14	2:C:3402:ERY:C30	2.29	0.61
1:A:216:ALA:HB2	1:B:750:LEU:HD13	1.83	0.61
1:C:363:ARG:HB3	1:C:496:MET:HB2	1.83	0.61
1:A:746:ILE:HG22	1:A:747:ASN:N	2.16	0.60
1:B:456:MET:CG	1:B:467:TYR:HB3	2.14	0.60
1:A:124:GLN:HG2	1:A:758:TYR:CE2	2.36	0.60
1:A:298:ASN:HD22	1:A:300:LEU:H	1.47	0.60
1:C:672:VAL:HG21	1:C:676:THR:H	1.66	0.60
1:B:10:ILE:HG13	1:C:893:GLU:O	2.01	0.60
1:A:965:LEU:O	1:A:969:ARG:HG3	2.01	0.60
1:B:28:LEU:HD12	1:B:29:LYS:HG3	1.82	0.60
1:C:958:LYS:HB3	1:C:962:GLU:CB	2.32	0.60
1:A:750:LEU:O	1:A:754:TRP:CD1	2.51	0.60
1:C:672:VAL:HG12	1:C:673:GLU:N	2.16	0.60
1:C:673:GLU:O	1:C:674:LEU:HB3	2.01	0.60
1:A:552:MET:HE3	1:A:906:PRO:HB3	1.83	0.60
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.37	0.60
1:A:56:THR:O	1:A:60:THR:HB	2.01	0.60
1:B:680:PHE:HD1	1:B:859:TRP:HZ3	1.50	0.60
1:B:139:VAL:HG12	1:B:139:VAL:O	2.00	0.60
1:A:246:PHE:O	1:A:249:ILE:CG1	2.47	0.60
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.02	0.60
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.83	0.60
1:C:419:VAL:HG23	1:C:430:ALA:HB1	1.84	0.60
1:B:699:ARG:HG2	1:B:700:ASN:H	1.67	0.60
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.36	0.60
1:B:456:MET:HG2	1:B:457:ALA:N	2.17	0.60
1:B:224:PRO:CA	1:C:781:MET:HE3	2.31	0.60
1:A:218:GLN:HB3	1:A:231:ASN:HD21	1.67	0.60
1:C:220:GLY:HA3	1:C:231:ASN:ND2	2.17	0.60
1:B:575:MET:HA	1:B:626:ILE:HG22	1.83	0.60
1:C:355:MET:HB3	1:C:365:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:930:GLY:HA3	1:C:1007:VAL:CG2	2.25	0.60
1:A:362:PHE:CZ	1:A:366:LEU:HD13	2.36	0.60
1:C:930:GLY:CA	1:C:1007:VAL:HG22	2.27	0.59
1:A:921:LEU:HG	1:A:922:THR:N	2.17	0.59
1:C:358:PHE:HB3	1:C:977:MET:HE1	1.82	0.59
1:C:322:LYS:HG2	1:C:323:ILE:O	2.02	0.59
1:C:713:LEU:HB2	1:C:832:ALA:HB3	1.84	0.59
1:B:911:GLY:HA3	1:B:1013:THR:HG21	1.83	0.59
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.84	0.59
1:A:617:PHE:CE2	1:A:666:PHE:HZ	2.20	0.59
1:B:225:VAL:HG11	1:C:778:LYS:HB3	1.84	0.59
1:A:243:THR:O	1:A:268:ILE:HG21	2.02	0.59
1:B:1022:VAL:CG2	1:B:1023:PRO:HD3	2.31	0.59
1:B:957:GLY:O	1:B:958:LYS:HG3	2.02	0.59
1:C:932:LEU:HA	1:C:935:ILE:CG2	2.31	0.59
1:C:156:ASP:HA	1:C:181:GLN:HA	1.84	0.59
1:C:882:ILE:HG22	1:C:882:ILE:O	2.03	0.59
1:B:703:LEU:HD12	1:B:716:VAL:HG12	1.84	0.59
1:B:68:ASN:O	1:B:70:ASN:N	2.36	0.59
1:C:961:ILE:O	1:C:965:LEU:HB2	2.02	0.59
1:C:608:SER:HB3	1:C:630:SER:HB2	1.84	0.59
1:C:899:PHE:N	1:C:899:PHE:HD1	2.00	0.59
1:C:1016:VAL:HA	1:C:1019:ILE:HG22	1.85	0.59
1:A:533:GLY:O	1:A:535:LEU:HG	2.02	0.59
1:C:354:VAL:HG12	1:C:354:VAL:O	2.02	0.59
1:B:370:ILE:O	1:B:370:ILE:HG22	2.02	0.59
1:B:184:MET:H	1:B:762:PHE:HE2	1.50	0.59
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.31	0.59
1:B:364:ALA:CB	1:B:497:LEU:HG	2.32	0.59
1:A:620:ARG:HG2	1:A:620:ARG:HH11	1.68	0.59
1:B:258:SER:O	1:B:259:ARG:HG2	2.03	0.59
1:B:235:ILE:CD1	1:B:235:ILE:N	2.65	0.58
1:B:225:VAL:H	1:C:781:MET:CE	2.16	0.58
1:B:213:GLN:HB2	1:B:239:ARG:CD	2.31	0.58
1:A:543:VAL:O	1:A:545:TYR:N	2.32	0.58
1:B:729:ILE:HG12	1:B:730:ASP:H	1.68	0.58
1:C:1:MET:HG3	1:C:3:ASN:H	1.68	0.58
1:B:345:VAL:HA	1:B:348:ILE:HD12	1.85	0.58
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.85	0.58
1:B:197:GLN:HA	1:B:798:MET:SD	2.43	0.58
1:B:355:MET:O	1:B:365:THR:OG1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:THR:HG21	1:B:833:PRO:HD2	1.84	0.58
1:C:155:SER:OG	1:C:179:GLY:HA3	2.02	0.58
1:B:426:PRO:HB3	1:B:430:ALA:CB	2.32	0.58
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.85	0.58
1:C:149:MET:SD	1:C:321:LEU:HD23	2.44	0.58
1:B:23:GLY:N	1:B:381:ALA:HB2	2.18	0.58
1:C:527:TYR:HE2	1:C:968:VAL:O	1.86	0.58
1:B:13:TRP:CE3	1:B:13:TRP:HA	2.37	0.58
1:A:543:VAL:HG22	1:A:544:LEU:H	1.68	0.58
1:C:331:PRO:O	1:C:335:ILE:HG12	2.04	0.58
1:B:99:ASP:OD2	1:B:99:ASP:C	2.40	0.58
1:A:5:PHE:CD1	1:A:12:ALA:HB2	2.38	0.58
1:A:212:ALA:O	1:A:213:GLN:HB2	2.02	0.58
1:A:240:LEU:HD23	1:A:246:PHE:HA	1.86	0.58
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.85	0.58
1:B:268:ILE:HD12	1:B:268:ILE:H	1.68	0.58
1:B:55:LYS:HD3	1:B:55:LYS:C	2.25	0.58
1:C:144:ASN:HA	1:C:320:GLY:O	2.04	0.58
1:B:371:ALA:HA	1:B:374:VAL:HG12	1.86	0.58
1:B:115:MET:HE1	1:B:127:VAL:HG21	1.84	0.58
1:C:463:THR:C	1:C:465:ALA:H	2.07	0.58
1:B:193:LEU:CD1	1:B:198:LEU:O	2.52	0.58
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.22	0.58
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.84	0.57
1:A:888:LEU:HD11	1:A:943:ILE:HG12	1.86	0.57
1:A:1021:PHE:HD1	1:A:1025:PHE:HE1	1.52	0.57
1:C:986:VAL:O	1:C:990:VAL:HG23	2.03	0.57
1:B:728:LYS:HG2	1:B:808:ARG:HD3	1.86	0.57
1:A:10:ILE:HD12	1:A:10:ILE:O	2.04	0.57
1:A:75:LEU:HD13	1:A:92:LEU:HB3	1.87	0.57
1:C:489:THR:O	1:C:493:CYS:HB3	2.03	0.57
1:A:348:ILE:HD11	1:A:372:VAL:CG1	2.33	0.57
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.86	0.57
1:C:674:LEU:HD13	1:C:862:MET:HA	1.85	0.57
1:C:907:LEU:HD22	1:C:1017:LEU:HD23	1.86	0.57
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.34	0.57
1:C:643:LYS:NZ	1:C:997:SER:HB2	2.20	0.57
1:C:685:ILE:O	1:C:687:GLN:HG2	2.05	0.57
1:A:1035:ARG:HH11	1:A:1035:ARG:HA	1.69	0.57
1:C:554:TYR:O	1:C:556:PHE:N	2.29	0.57
1:B:345:VAL:C	1:B:347:ALA:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:SER:O	1:B:983:ILE:HG12	2.03	0.57
1:A:820:ASN:ND2	3:A:4001:HOH:O	2.33	0.57
1:B:398:MET:HG3	1:B:473:THR:HG21	1.87	0.57
1:B:57:VAL:CG1	1:B:58:GLN:N	2.67	0.57
1:C:146:ASP:C	1:C:148:THR:H	2.08	0.57
1:C:672:VAL:CG1	1:C:673:GLU:N	2.63	0.57
1:A:659:LYS:NZ	1:A:660:ASP:O	2.38	0.57
1:C:144:ASN:HD21	1:C:148:THR:N	2.02	0.57
1:A:882:ILE:O	1:A:886:LEU:HB2	2.05	0.57
1:B:673:GLU:O	1:B:676:THR:CG2	2.51	0.57
1:B:349:ILE:O	1:B:351:VAL:N	2.36	0.57
1:C:899:PHE:CD1	1:C:899:PHE:N	2.72	0.57
1:B:425:LEU:HB2	1:B:498:LYS:O	2.04	0.57
1:A:216:ALA:CB	1:B:750:LEU:HD13	2.35	0.57
1:A:456:MET:O	1:A:458:PHE:N	2.35	0.57
1:C:681:ASP:HB3	1:C:860:THR:HG23	1.87	0.57
1:C:395:MET:HE2	1:C:395:MET:HA	1.87	0.57
1:C:88:VAL:HG12	1:C:90:ILE:HD12	1.86	0.57
1:B:792:ARG:HG2	1:B:793:ALA:H	1.70	0.57
1:B:453:PHE:HZ	1:B:933:THR:HG23	1.69	0.56
1:C:400:LEU:HD12	1:C:929:VAL:CG1	2.35	0.56
1:A:871:ASN:O	1:A:874:PRO:HD2	2.04	0.56
1:C:184:MET:HG2	1:C:246:PHE:CD1	2.40	0.56
1:A:5:PHE:HD1	1:A:12:ALA:HB2	1.68	0.56
1:A:723:ASP:OD1	1:A:813:SER:N	2.38	0.56
1:B:537:SER:O	1:B:539:GLY:N	2.38	0.56
1:B:900:SER:HB2	1:B:1026:PHE:CZ	2.40	0.56
1:B:934:THR:C	1:B:936:GLY:N	2.58	0.56
1:C:13:TRP:O	1:C:17:ILE:HG12	2.06	0.56
1:A:199:THR:CG2	1:A:791:VAL:HA	2.35	0.56
1:C:159:ALA:CB	1:C:181:GLN:HB2	2.35	0.56
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.40	0.56
1:B:298:ASN:ND2	1:B:301:ASP:OD1	2.39	0.56
1:A:911:GLY:H	1:A:914:LEU:HD13	1.70	0.56
1:A:880:SER:O	1:A:884:VAL:HG23	2.06	0.56
1:B:314:GLU:HG2	1:B:317:PHE:CE2	2.40	0.56
1:B:743:ILE:H	1:B:743:ILE:CD1	2.09	0.56
1:B:149:MET:CB	1:B:154:ILE:HG22	2.35	0.56
1:B:213:GLN:HB2	1:B:239:ARG:CG	2.34	0.56
1:C:48:SER:HB2	1:C:87:THR:HG22	1.87	0.56
1:B:36:PRO:HD2	1:B:38:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:LEU:HD21	1:B:1023:PRO:HB2	1.87	0.56
1:B:539:GLY:C	1:B:541:TYR:H	2.07	0.56
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.40	0.56
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.20	0.56
1:A:204:ILE:CD1	1:A:773:VAL:HG11	2.35	0.56
1:C:947:GLU:C	1:C:949:ALA:H	2.09	0.56
1:B:921:LEU:HD21	1:B:1002:ALA:HA	1.87	0.56
1:B:589:LYS:HA	1:B:592:ASN:OD1	2.05	0.56
1:C:228:GLN:NE2	1:C:230:LEU:O	2.39	0.56
1:A:747:ASN:HD21	1:C:237:GLN:NE2	2.04	0.56
1:B:356:TYR:HE2	1:B:365:THR:HG21	1.70	0.56
1:A:600:THR:O	1:A:601:LYS:HB2	2.06	0.56
1:B:73:ASP:HB2	1:B:106:GLN:HE22	1.71	0.56
1:C:20:MET:O	1:C:377:LEU:HD12	2.06	0.56
1:C:367:ILE:HD11	1:C:489:THR:HA	1.87	0.56
1:A:527:TYR:CE2	1:A:972:LEU:HG	2.41	0.56
1:A:70:ASN:HB3	1:C:167:SER:HB3	1.88	0.56
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.88	0.56
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.41	0.56
1:C:100:ALA:HB2	1:C:295:THR:HG21	1.88	0.56
1:C:958:LYS:HB3	1:C:962:GLU:HB3	1.87	0.55
1:C:1016:VAL:C	1:C:1018:ALA:H	2.09	0.55
1:B:445:ILE:HD13	1:B:943:ILE:CG2	2.36	0.55
1:A:240:LEU:N	1:A:240:LEU:HD12	2.20	0.55
1:B:23:GLY:HA2	1:B:26:ALA:HB3	1.89	0.55
1:C:818:ARG:HA	1:C:824:SER:H	1.71	0.55
1:A:1029:VAL:O	1:A:1030:ARG:HB2	2.05	0.55
1:A:582:ALA:HB3	1:A:623:ASN:HB2	1.88	0.55
1:C:655:PHE:C	1:C:657:GLN:H	2.09	0.55
1:B:778:LYS:H	1:B:778:LYS:HD3	1.71	0.55
1:A:4:PHE:HB3	1:A:8:ARG:HH21	1.72	0.55
1:B:231:ASN:ND2	1:B:231:ASN:C	2.60	0.55
1:C:713:LEU:HG	1:C:833:PRO:C	2.27	0.55
1:B:881:LEU:HD21	1:B:905:VAL:HG21	1.89	0.55
1:C:351:VAL:O	1:C:355:MET:HB2	2.07	0.55
1:B:892:TYR:CB	1:B:897:ILE:HD11	2.37	0.55
1:B:366:LEU:O	1:B:369:THR:N	2.36	0.55
1:B:224:PRO:HA	1:C:781:MET:CE	2.36	0.55
2:C:3402:ERY:C14	2:C:3402:ERY:C30	2.84	0.55
1:B:712:MET:HA	1:B:834:GLY:HA3	1.87	0.55
1:B:680:PHE:CD1	1:B:859:TRP:HZ3	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:LEU:C	1:C:355:MET:H	2.10	0.55
1:B:847:LEU:O	1:B:850:LYS:HG2	2.06	0.55
1:C:1032:ARG:HB3	1:C:1032:ARG:HH21	1.71	0.55
1:C:57:VAL:HG12	1:C:88:VAL:HG22	1.88	0.55
1:A:617:PHE:CE2	1:A:626:ILE:HD11	2.42	0.55
1:B:1023:PRO:O	1:B:1027:VAL:HG22	2.07	0.55
1:C:837:THR:O	1:C:841:MET:HG3	2.07	0.55
1:A:688:ALA:O	1:A:690:LEU:N	2.38	0.55
1:C:211:ASN:HA	1:C:240:LEU:HD23	1.89	0.55
1:A:574:THR:HB	1:A:627:ALA:HB3	1.87	0.55
1:C:692:HIS:CE1	1:C:721:LEU:HD21	2.30	0.55
1:B:987:MET:N	1:B:988:PRO:HD2	2.22	0.55
1:B:415:ASN:ND2	1:B:434:SER:OG	2.36	0.55
1:A:156:ASP:OD1	1:A:182:TYR:HB2	2.07	0.55
1:B:709:HIS:N	1:B:710:PRO:HD3	2.22	0.55
1:A:4:PHE:O	1:A:8:ARG:HG2	2.08	0.54
1:B:13:TRP:HE3	1:B:13:TRP:HA	1.70	0.54
1:A:216:ALA:HA	1:B:751:GLY:HA2	1.89	0.54
1:B:768:VAL:HG23	1:C:63:GLN:NE2	2.22	0.54
1:B:240:LEU:O	1:B:762:PHE:HB2	2.07	0.54
1:A:219:LEU:HD22	1:B:781:MET:O	2.06	0.54
1:B:247:GLY:HA2	1:B:268:ILE:HD13	1.88	0.54
1:C:489:THR:N	1:C:490:PRO:HD2	2.22	0.54
1:A:418:ARG:HA	1:A:421:ALA:HB3	1.90	0.54
1:B:927:PHE:CE1	1:B:931:LEU:HG	2.42	0.54
1:A:991:ILE:O	1:A:992:SER:HB3	2.07	0.54
1:B:59:ASP:HA	1:B:63:GLN:CG	2.37	0.54
1:C:607:GLU:HB2	1:C:632:LYS:CG	2.36	0.54
1:C:632:LYS:O	1:C:634:TRP:N	2.39	0.54
1:A:703:LEU:HD11	1:A:718:PRO:HD3	1.88	0.54
1:A:609:VAL:HG12	1:A:629:VAL:HB	1.89	0.54
1:B:219:LEU:HD23	1:B:230:LEU:HD11	1.88	0.54
1:B:971:ARG:HA	1:B:974:PRO:HG2	1.89	0.54
1:B:250:LEU:HA	1:B:261:LEU:HB3	1.88	0.54
1:C:909:VAL:HA	1:C:931:LEU:HD11	1.88	0.54
1:C:326:PRO:HG3	1:C:610:PHE:CD1	2.43	0.54
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.89	0.54
1:B:913:LEU:O	1:B:917:THR:HB	2.08	0.54
1:A:126:GLY:HA3	1:B:116:PRO:HB3	1.89	0.54
1:A:699:ARG:HH22	1:A:722:GLU:CD	2.10	0.54
1:B:274:ASN:OD1	1:B:276:ASP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:732:ASP:O	1:C:733:GLN:C	2.45	0.54
1:C:819:TYR:N	1:C:824:SER:HB3	2.23	0.54
1:B:569:GLN:HE21	1:B:668:LEU:HB2	1.71	0.54
1:C:9:PRO:HG3	1:C:491:ALA:HB1	1.89	0.54
1:C:912:ALA:C	1:C:914:LEU:H	2.11	0.54
1:C:142:VAL:HG12	1:C:154:ILE:CG2	2.38	0.54
1:C:1018:ALA:O	1:C:1022:VAL:HG12	2.08	0.54
1:A:302:THR:O	1:A:306:ILE:HG12	2.08	0.54
1:B:773:VAL:CG1	1:B:773:VAL:O	2.56	0.54
1:C:203:VAL:HG13	1:C:262:LEU:HD11	1.89	0.54
1:B:767:ARG:HA	1:C:63:GLN:HE22	1.73	0.54
1:A:133:SER:O	1:A:135:SER:N	2.32	0.54
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.29	0.53
1:B:699:ARG:O	1:B:701:GLN:N	2.40	0.53
1:C:938:SER:O	1:C:941:ASN:ND2	2.41	0.53
1:C:782:LEU:HB3	1:C:783:PRO:HD2	1.90	0.53
1:B:892:TYR:O	1:B:894:SER:N	2.42	0.53
1:C:415:ASN:O	1:C:418:ARG:HG2	2.07	0.53
1:B:115:MET:HA	1:B:115:MET:CE	2.37	0.53
1:C:839:GLU:HA	1:C:842:GLU:CB	2.38	0.53
1:B:16:ALA:HB2	1:B:488:LEU:HG	1.90	0.53
1:B:777:ALA:O	1:B:781:MET:HE2	2.08	0.53
1:B:158:VAL:HA	1:B:162:MET:HG2	1.90	0.53
1:A:248:LYS:HA	1:A:261:LEU:HD22	1.90	0.53
1:A:83:ASP:HB3	1:A:815:ARG:HG3	1.89	0.53
1:B:1017:LEU:O	1:B:1021:PHE:HD2	1.92	0.53
1:A:313:MET:HB2	1:A:317:PHE:CE1	2.44	0.53
1:A:754:TRP:CE3	1:A:780:ARG:HB2	2.44	0.53
1:C:601:LYS:C	1:C:603:LYS:H	2.11	0.53
1:A:781:MET:CE	1:C:228:GLN:OE1	2.56	0.53
1:A:740:GLY:HA3	1:A:794:ALA:H	1.73	0.53
1:C:594:VAL:HG13	1:C:598:TYR:HE1	1.73	0.53
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.43	0.53
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.90	0.53
1:C:265:VAL:O	1:C:265:VAL:CG2	2.50	0.53
1:C:444:GLY:O	1:C:448:VAL:HG23	2.08	0.53
1:C:358:PHE:HB3	1:C:977:MET:CE	2.39	0.53
1:C:371:ALA:HB2	1:C:488:LEU:HD23	1.90	0.53
1:A:987:MET:N	1:A:988:PRO:CD	2.72	0.53
1:B:428:LYS:O	1:B:432:ARG:HG3	2.07	0.53
1:B:152:GLU:O	1:B:182:TYR:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:VAL:O	1:B:453:PHE:HB2	2.08	0.53
1:B:580:ALA:O	1:B:582:ALA:N	2.41	0.53
1:B:393:LEU:HB2	1:B:469:GLN:HG2	1.89	0.53
1:C:945:ILE:C	1:C:947:GLU:H	2.12	0.53
1:B:120:GLN:O	1:B:124:GLN:HG2	2.08	0.53
1:B:1005:THR:HG22	1:B:1005:THR:O	2.09	0.53
1:C:761:ASP:HB3	1:C:769:LYS:O	2.09	0.53
1:B:252:LYS:HB3	1:B:260:VAL:HG12	1.91	0.53
1:B:344:LEU:O	1:B:347:ALA:HB3	2.09	0.53
1:C:60:THR:HG22	1:C:61:VAL:HG23	1.89	0.53
1:A:351:VAL:O	1:A:355:MET:HB2	2.08	0.53
1:B:339:GLU:HA	1:B:339:GLU:OE1	2.08	0.53
1:A:578:LEU:HD21	1:A:587:THR:HA	1.91	0.53
1:B:528:THR:O	1:B:531:VAL:HG12	2.08	0.53
1:C:164:ASP:O	1:C:168:ARG:HG3	2.09	0.53
1:C:655:PHE:HB3	1:C:663:VAL:CG2	2.38	0.53
1:B:888:LEU:HB2	1:B:898:PRO:HB3	1.90	0.53
1:A:35:TYR:CD1	1:A:671:ILE:HG22	2.44	0.53
1:B:445:ILE:HG23	1:B:940:LYS:CG	2.29	0.53
1:B:393:LEU:HD13	1:B:466:ILE:HG23	1.90	0.53
1:C:851:LEU:HB3	1:C:852:PRO:HD2	1.91	0.53
1:A:242:SER:HB3	1:A:245:GLU:HB2	1.91	0.53
1:A:164:ASP:HA	1:A:167:SER:HB2	1.91	0.53
1:A:128:SER:HB2	1:B:113:LEU:HD23	1.90	0.53
1:B:399:VAL:HG11	1:B:989:LEU:HG	1.90	0.53
1:A:152:GLU:HG2	1:A:272:GLY:HA3	1.91	0.53
1:C:591:LEU:HD12	1:C:611:ALA:HB1	1.89	0.53
1:C:400:LEU:HD21	1:C:1003:VAL:HG13	1.91	0.52
1:B:986:VAL:CG2	1:B:1008:MET:HB2	2.38	0.52
1:A:947:GLU:O	1:A:951:ASP:N	2.40	0.52
1:B:564:LEU:HD23	1:B:565:PRO:HD2	1.90	0.52
1:B:1:MET:HG2	1:B:439:GLN:HE22	1.74	0.52
1:C:350:LEU:HD21	1:C:984:LEU:HD22	1.90	0.52
1:A:235:ILE:O	1:A:235:ILE:HG22	2.09	0.52
1:B:57:VAL:HG12	1:B:58:GLN:H	1.74	0.52
1:C:466:ILE:HG13	1:C:563:PHE:HZ	1.73	0.52
1:C:172:VAL:HG22	1:C:306:ILE:HD11	1.91	0.52
1:B:434:SER:O	1:B:438:ILE:HG22	2.10	0.52
1:C:997:SER:O	1:C:999:ALA:N	2.43	0.52
1:B:409:ALA:HA	1:B:485:ALA:HB2	1.90	0.52
1:A:193:LEU:HB2	1:A:265:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:VAL:HG11	1:A:591:LEU:CD2	2.39	0.52
1:B:867:ARG:HG2	1:B:868:LEU:HD22	1.91	0.52
1:C:907:LEU:HD13	1:C:1018:ALA:HA	1.90	0.52
1:C:348:ILE:C	1:C:350:LEU:H	2.11	0.52
1:B:185:ARG:HD2	1:B:772:TYR:HB2	1.91	0.52
1:C:884:VAL:C	1:C:886:LEU:H	2.13	0.52
1:B:2:PRO:HB3	1:B:486:LEU:O	2.09	0.52
1:A:214:VAL:HG21	1:B:747:ASN:ND2	2.24	0.52
1:C:445:ILE:O	1:C:449:LEU:N	2.39	0.52
1:B:190:PRO:HB3	1:B:789:TRP:CD2	2.45	0.52
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.92	0.52
1:B:942:ALA:HA	1:B:1022:VAL:HG11	1.90	0.52
1:C:641:GLU:H	1:C:641:GLU:CD	2.13	0.52
1:C:911:GLY:HA3	1:C:1010:GLY:HA2	1.91	0.52
1:C:831:ALA:HB2	1:C:840:ALA:CB	2.40	0.52
1:C:899:PHE:H	1:C:899:PHE:HD1	1.57	0.52
1:B:5:PHE:O	1:B:9:PRO:HA	2.08	0.52
1:C:208:LYS:HA	1:C:760:ASN:HD21	1.75	0.52
1:A:395:MET:HA	1:A:395:MET:CE	2.40	0.52
1:B:204:ILE:HG23	1:B:759:VAL:HG13	1.92	0.52
1:B:193:LEU:HD11	1:B:198:LEU:O	2.09	0.52
1:C:527:TYR:OH	1:C:1019:ILE:HG13	2.09	0.52
1:B:13:TRP:HD1	1:C:895:TRP:HZ2	1.57	0.52
1:A:584:GLN:H	1:A:622:GLN:HG2	1.74	0.52
1:A:200:PRO:HA	1:A:203:VAL:HG23	1.92	0.52
1:C:378:GLY:O	1:C:382:VAL:HG23	2.10	0.52
1:A:406:VAL:HG12	1:A:407:ASP:N	2.24	0.52
1:C:646:ALA:HA	1:C:649:MET:HB2	1.92	0.52
1:B:115:MET:HA	1:B:118:LEU:HD13	1.92	0.52
1:C:169:THR:O	1:C:172:VAL:HG23	2.10	0.52
1:A:688:ALA:C	1:A:690:LEU:H	2.12	0.52
1:A:62:THR:HG23	1:A:88:VAL:CG1	2.40	0.52
1:B:52:ALA:HB2	1:B:85:THR:C	2.29	0.52
1:C:124:GLN:HB3	1:C:758:TYR:HE2	1.74	0.52
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.43	0.52
1:B:972:LEU:HD21	1:B:1019:ILE:HG12	1.91	0.52
1:C:736:ALA:C	1:C:738:ALA:H	2.12	0.52
1:B:45:ILE:HB	1:B:90:ILE:HB	1.92	0.52
1:B:459:PHE:O	1:B:464:GLY:HA3	2.10	0.52
1:B:911:GLY:HA2	1:B:914:LEU:CB	2.40	0.52
1:C:923:ASN:HD22	1:C:927:PHE:HD2	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:VAL:O	1:C:226:LYS:C	2.48	0.52
1:C:402:ILE:O	1:C:406:VAL:HG23	2.10	0.52
1:B:873:ALA:HB1	1:B:877:TYR:CE2	2.45	0.52
1:B:1026:PHE:HB3	1:B:1030:ARG:HE	1.74	0.51
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.91	0.51
1:A:525:HIS:HA	1:A:528:THR:CG2	2.37	0.51
1:C:615:PHE:C	1:C:615:PHE:CD2	2.83	0.51
1:C:527:TYR:OH	1:C:968:VAL:HG12	2.10	0.51
1:B:699:ARG:HA	1:B:702:LEU:HB2	1.92	0.51
1:B:729:ILE:CG1	1:B:730:ASP:H	2.23	0.51
1:C:395:MET:O	1:C:398:MET:N	2.43	0.51
1:A:324:VAL:HG12	1:A:325:TYR:H	1.75	0.51
1:C:68:ASN:N	1:C:68:ASN:OD1	2.43	0.51
1:C:34:GLN:O	1:C:391:ASN:HB2	2.09	0.51
1:A:886:LEU:HD12	1:C:14:VAL:HG23	1.90	0.51
1:B:482:VAL:O	1:B:486:LEU:HB2	2.10	0.51
1:A:550:VAL:O	1:A:553:ALA:N	2.43	0.51
1:B:280:GLU:CB	1:B:284:GLN:O	2.58	0.51
1:B:897:ILE:HG13	1:B:898:PRO:HD3	1.92	0.51
1:A:945:ILE:HG13	1:A:971:ARG:CG	2.27	0.51
1:B:291:ILE:HG21	1:B:306:ILE:HD11	1.91	0.51
1:B:754:TRP:HH2	1:B:785:ASP:HB2	1.76	0.51
1:C:210:GLN:O	1:C:240:LEU:CD2	2.58	0.51
1:C:176:GLN:HE22	1:C:620:ARG:HH12	1.58	0.51
1:B:776:GLU:HG2	1:B:777:ALA:H	1.75	0.51
1:A:204:ILE:HD11	1:A:773:VAL:HG11	1.93	0.51
1:A:63:GLN:O	1:A:64:VAL:C	2.48	0.51
1:C:731:ILE:HD13	1:C:746:ILE:HG21	1.92	0.51
1:C:102:ILE:O	1:C:103:ALA:C	2.47	0.51
1:A:886:LEU:HD13	1:C:14:VAL:HG23	1.91	0.51
1:C:681:ASP:CB	1:C:860:THR:CG2	2.83	0.51
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.25	0.51
1:B:13:TRP:O	1:B:16:ALA:HB3	2.11	0.51
1:C:326:PRO:CB	1:C:610:PHE:HB2	2.40	0.51
1:A:139:VAL:CG1	1:A:327:TYR:HB3	2.39	0.51
1:B:418:ARG:HH11	1:B:418:ARG:HB3	1.76	0.51
1:C:423:GLU:CB	1:C:426:PRO:HD2	2.41	0.51
1:A:431:THR:O	1:A:435:MET:HB2	2.11	0.51
1:A:196:PHE:CG	1:A:260:VAL:HG11	2.45	0.51
1:A:282:ASN:ND2	1:A:609:VAL:H	2.08	0.51
1:B:428:LYS:CB	1:B:494:ALA:HB1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:SER:HA	1:A:175:VAL:HG21	1.93	0.51
1:A:584:GLN:N	1:A:622:GLN:HG2	2.25	0.51
1:A:671:ILE:CG1	1:A:674:LEU:HB3	2.41	0.51
1:C:465:ALA:O	1:C:469:GLN:HG2	2.10	0.51
1:C:712:MET:HB2	1:C:839:GLU:OE1	2.11	0.51
1:C:176:GLN:HE21	1:C:620:ARG:HH11	1.55	0.51
1:A:601:LYS:O	1:A:602:GLU:HG2	2.11	0.51
1:C:326:PRO:HB3	1:C:610:PHE:HB2	1.93	0.51
1:A:585:GLU:OE2	1:C:227:GLY:HA2	2.10	0.51
1:C:352:PHE:HA	1:C:369:THR:HG21	1.93	0.51
1:C:404:LEU:HD21	1:C:449:LEU:CD1	2.41	0.51
1:C:181:GLN:CG	1:C:769:LYS:HE2	2.41	0.51
1:B:213:GLN:HE21	1:B:239:ARG:HD2	1.76	0.51
1:B:68:ASN:O	1:B:70:ASN:ND2	2.44	0.51
1:B:683:GLU:O	1:B:857:TYR:HA	2.10	0.51
1:C:801:PHE:CD1	1:C:804:PHE:CE1	2.99	0.51
1:B:160:ALA:HB1	1:B:767:ARG:HD3	1.93	0.51
1:A:261:LEU:CD1	1:A:263:ARG:HH11	2.24	0.51
1:C:239:ARG:HB2	1:C:763:ILE:CD1	2.41	0.51
1:B:900:SER:HA	1:B:903:LEU:HD12	1.92	0.50
1:B:552:MET:SD	1:B:909:VAL:HG23	2.50	0.50
1:B:764:ASP:HB3	1:B:769:LYS:HE3	1.93	0.50
1:C:485:ALA:HA	1:C:489:THR:OG1	2.11	0.50
1:A:455:PRO:HG2	1:A:880:SER:HB2	1.91	0.50
1:A:819:TYR:N	1:A:824:SER:HB3	2.25	0.50
1:B:899:PHE:O	1:B:899:PHE:CD1	2.64	0.50
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.92	0.50
1:B:49:TYR:HB3	1:B:57:VAL:HG23	1.92	0.50
1:B:46:SER:HA	1:B:88:VAL:O	2.12	0.50
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.93	0.50
1:A:780:ARG:HG2	1:A:780:ARG:NH1	2.25	0.50
1:B:213:GLN:HE21	1:B:239:ARG:CD	2.25	0.50
1:A:92:LEU:H	1:A:92:LEU:HD12	1.75	0.50
1:B:539:GLY:C	1:B:541:TYR:N	2.64	0.50
1:A:185:ARG:HD3	1:A:272:GLY:O	2.10	0.50
1:B:282:ASN:O	1:B:284:GLN:N	2.44	0.50
1:C:76:MET:SD	1:C:95:GLU:HG3	2.51	0.50
1:C:463:THR:HA	1:C:466:ILE:HG12	1.93	0.50
1:C:144:ASN:ND2	1:C:149:MET:N	2.57	0.50
1:C:189:ASN:ND2	1:C:192:GLU:H	2.09	0.50
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:876:LEU:HD22	1:B:932:LEU:HD13	1.93	0.50
1:B:59:ASP:HA	1:B:63:GLN:HG2	1.93	0.50
1:A:781:MET:HE1	1:C:225:VAL:H	1.77	0.50
1:C:946:VAL:O	1:C:946:VAL:HG12	2.12	0.50
1:C:631:LEU:HB3	1:C:637:ARG:NH2	2.27	0.50
1:C:588:GLN:HG2	1:C:613:ASN:ND2	2.25	0.50
1:C:47:ALA:HB2	1:C:127:VAL:HG12	1.92	0.50
1:C:382:VAL:HG11	1:C:476:SER:HB2	1.94	0.50
1:A:877:TYR:O	1:A:881:LEU:HB2	2.12	0.50
1:B:891:LEU:HD12	1:B:892:TYR:CE1	2.46	0.50
1:A:659:LYS:CG	1:A:660:ASP:H	2.05	0.50
1:A:612:VAL:CG2	1:A:626:ILE:HG22	2.37	0.50
1:B:261:LEU:O	1:B:263:ARG:N	2.44	0.50
1:B:714:THR:HG21	1:B:832:ALA:H	1.75	0.50
1:A:578:LEU:CD2	1:A:587:THR:HG23	2.42	0.50
1:A:36:PRO:HG3	1:A:469:GLN:OE1	2.12	0.50
1:B:251:LEU:HB2	1:B:261:LEU:HA	1.94	0.50
1:B:213:GLN:HG3	1:C:56:THR:CG2	2.41	0.50
1:C:734:GLU:HA	1:C:737:GLN:HE21	1.76	0.50
1:C:912:ALA:O	1:C:914:LEU:N	2.44	0.50
1:B:699:ARG:HB3	1:B:699:ARG:HH11	1.77	0.50
1:C:239:ARG:HB2	1:C:763:ILE:HD13	1.92	0.50
1:B:814:PRO:O	1:B:815:ARG:HG2	2.12	0.50
1:C:920:GLY:O	1:C:921:LEU:O	2.28	0.50
1:C:477:ALA:HA	1:C:480:LEU:HB2	1.93	0.50
1:B:30:LEU:HD12	1:B:384:ALA:HB2	1.92	0.50
1:A:904:VAL:HA	1:A:907:LEU:HD13	1.94	0.50
1:B:391:ASN:HD21	1:B:393:LEU:HB2	1.77	0.50
1:B:964:THR:O	1:B:968:VAL:HG23	2.11	0.50
1:B:158:VAL:HB	1:B:289:LEU:HD21	1.93	0.50
1:A:677:ALA:O	1:A:679:GLY:N	2.31	0.50
1:B:990:VAL:HG13	1:B:1005:THR:OG1	2.10	0.50
1:B:261:LEU:HD23	1:B:261:LEU:O	2.12	0.50
1:B:135:SER:HB2	1:B:676:THR:CG2	2.42	0.50
1:B:905:VAL:HG13	1:B:906:PRO:CD	2.40	0.50
1:A:159:ALA:HB2	1:A:177:LEU:HD22	1.93	0.50
1:B:428:LYS:HB2	1:B:494:ALA:HB1	1.93	0.50
1:B:323:ILE:HD12	1:B:323:ILE:N	2.27	0.50
1:A:841:MET:O	1:A:845:GLU:HG3	2.12	0.50
1:A:832:ALA:O	1:A:833:PRO:C	2.49	0.49
1:A:193:LEU:HD12	1:A:265:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.12	0.49
1:A:1022:VAL:HA	1:A:1025:PHE:HD1	1.77	0.49
1:A:543:VAL:C	1:A:545:TYR:N	2.65	0.49
1:B:729:ILE:HG12	1:B:730:ASP:N	2.25	0.49
1:A:201:VAL:HG21	1:A:745:ASP:OD2	2.12	0.49
1:A:66:GLU:C	1:A:68:ASN:H	2.15	0.49
1:A:583:THR:HG22	1:A:585:GLU:N	2.27	0.49
1:C:220:GLY:HA3	1:C:231:ASN:HD22	1.76	0.49
1:C:941:ASN:HD22	1:C:942:ALA:N	2.10	0.49
1:A:590:VAL:O	1:A:594:VAL:HG23	2.12	0.49
1:A:586:ARG:HA	1:A:589:LYS:HE3	1.94	0.49
1:A:311:ALA:O	1:A:312:LYS:HB2	2.11	0.49
1:C:1:MET:HB2	1:C:2:PRO:CD	2.38	0.49
1:B:741:VAL:HG12	1:B:792:ARG:O	2.12	0.49
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.76	0.49
1:A:979:SER:O	1:A:983:ILE:HG23	2.12	0.49
1:C:414:GLU:HA	1:C:417:GLU:HG2	1.95	0.49
1:A:187:TRP:HZ2	1:A:275:TYR:HE1	1.60	0.49
1:A:644:VAL:HG11	1:A:667:ASN:OD1	2.12	0.49
1:C:713:LEU:HD21	1:C:835:LYS:N	2.27	0.49
1:C:442:LEU:O	1:C:445:ILE:HG13	2.12	0.49
1:B:404:LEU:C	1:B:406:VAL:H	2.16	0.49
1:C:754:TRP:CZ3	1:C:780:ARG:HA	2.46	0.49
1:C:540:ARG:O	1:C:544:LEU:HB2	2.13	0.49
1:C:367:ILE:HG23	1:C:368:PRO:HD3	1.93	0.49
1:A:232:ALA:HB1	1:B:725:PRO:O	2.12	0.49
1:B:183:ALA:HB2	1:B:273:GLU:HB3	1.94	0.49
1:C:713:LEU:HD21	1:C:835:LYS:H	1.78	0.49
1:B:166:ILE:HD11	1:B:310:LEU:HG	1.94	0.49
1:B:164:ASP:HB3	1:B:168:ARG:HH22	1.78	0.49
1:C:26:ALA:O	1:C:30:LEU:HD12	2.12	0.49
1:C:726:GLN:CD	1:C:812:GLY:HA3	2.33	0.49
1:B:708:LYS:O	1:B:708:LYS:HG2	2.12	0.49
1:B:623:ASN:N	1:B:623:ASN:OD1	2.37	0.49
1:B:897:ILE:N	1:B:898:PRO:CD	2.76	0.49
1:A:708:LYS:C	1:A:710:PRO:HD3	2.33	0.49
1:B:95:GLU:O	1:B:98:THR:HG22	2.12	0.49
1:C:618:ALA:CB	1:C:815:ARG:HH12	2.23	0.49
1:C:681:ASP:HB3	1:C:860:THR:HG22	1.94	0.49
1:A:1:MET:SD	1:A:487:ILE:CD1	3.01	0.49
1:B:580:ALA:O	1:B:581:GLY:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:THR:HB	1:B:613:ASN:HD21	1.78	0.49
1:A:937:LEU:HD12	1:A:1011:MET:SD	2.53	0.49
1:C:456:MET:O	1:C:459:PHE:HB2	2.13	0.49
1:B:49:TYR:HB3	1:B:57:VAL:CG2	2.43	0.49
1:C:84:SER:C	1:C:86:GLY:N	2.65	0.49
1:C:894:SER:C	1:C:896:SER:H	2.16	0.49
1:B:764:ASP:O	1:B:766:GLY:N	2.39	0.49
1:B:831:ALA:CB	1:B:840:ALA:HB2	2.42	0.49
1:C:911:GLY:CA	1:C:1010:GLY:HA2	2.43	0.49
1:C:395:MET:HE2	1:C:395:MET:CA	2.42	0.49
1:A:416:VAL:HG22	1:A:434:SER:OG	2.12	0.49
1:C:952:LEU:O	1:C:953:MET:HG3	2.13	0.49
1:A:253:VAL:HG23	1:A:259:ARG:HG2	1.94	0.49
1:C:879:ILE:O	1:C:879:ILE:HG22	2.13	0.49
1:C:33:ALA:HB1	1:C:34:GLN:HE21	1.78	0.49
1:C:713:LEU:CD1	1:C:835:LYS:H	2.18	0.49
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.78	0.49
1:C:968:VAL:HG11	1:C:1023:PRO:HG3	1.94	0.49
1:B:16:ALA:O	1:B:374:VAL:HG23	2.13	0.49
1:B:1025:PHE:O	1:B:1029:VAL:HG12	2.13	0.49
1:C:349:ILE:O	1:C:349:ILE:HG23	2.13	0.49
1:A:561:SER:HA	1:A:923:ASN:HB3	1.95	0.49
1:B:154:ILE:O	1:B:157:TYR:N	2.46	0.48
1:C:590:VAL:O	1:C:592:ASN:O	2.30	0.48
1:C:75:LEU:HD11	1:C:92:LEU:HD23	1.95	0.48
1:C:975:ILE:HG21	1:C:1019:ILE:HD13	1.95	0.48
1:C:425:LEU:H	1:C:426:PRO:CD	2.26	0.48
1:A:191:ASN:C	1:A:193:LEU:N	2.67	0.48
1:A:376:LEU:C	1:A:378:GLY:H	2.14	0.48
1:A:783:PRO:C	1:A:785:ASP:H	2.17	0.48
1:B:776:GLU:HG2	1:B:777:ALA:N	2.28	0.48
1:C:1032:ARG:NH2	1:C:1032:ARG:HB3	2.29	0.48
1:A:467:TYR:CE1	1:A:925:VAL:HG13	2.47	0.48
1:A:649:MET:HA	1:A:653:ARG:HH22	1.76	0.48
1:A:173:GLY:N	1:A:293:LEU:O	2.43	0.48
1:A:316:PHE:CD2	1:A:316:PHE:N	2.82	0.48
1:B:946:VAL:HG21	1:B:1026:PHE:CE2	2.48	0.48
1:C:577:GLN:H	1:C:577:GLN:HE21	1.60	0.48
1:C:750:LEU:HD23	1:C:754:TRP:CD1	2.49	0.48
1:A:295:THR:HG22	1:A:295:THR:O	2.13	0.48
1:A:620:ARG:HG2	1:A:620:ARG:NH1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG21	1:B:747:ASN:CG	2.34	0.48
1:A:897:ILE:N	1:A:898:PRO:HD2	2.27	0.48
1:B:654:ALA:C	1:B:656:SER:H	2.16	0.48
1:A:660:ASP:O	1:A:661:ALA:HB2	2.12	0.48
1:A:947:GLU:O	1:A:951:ASP:HB2	2.13	0.48
1:C:681:ASP:HB2	1:C:860:THR:HG23	1.94	0.48
1:B:952:LEU:C	1:B:954:ASP:N	2.65	0.48
1:C:486:LEU:C	1:C:490:PRO:HG3	2.34	0.48
1:C:655:PHE:C	1:C:657:GLN:N	2.67	0.48
1:A:57:VAL:HG12	1:A:82:SER:HB3	1.96	0.48
1:A:52:ALA:HB3	1:A:86:GLY:HA2	1.95	0.48
1:B:157:TYR:C	1:B:161:ASN:HD22	2.16	0.48
1:B:989:LEU:HD13	1:B:1000:GLN:O	2.13	0.48
1:B:420:MET:HG2	1:B:426:PRO:HD3	1.95	0.48
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.76	0.48
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.93	0.48
1:A:45:ILE:HG23	1:A:129:VAL:CG2	2.43	0.48
1:B:219:LEU:CD1	1:B:234:ILE:HG12	2.44	0.48
1:B:744:ASN:O	1:B:748:THR:N	2.40	0.48
1:B:448:VAL:O	1:B:452:VAL:HG23	2.13	0.48
1:B:453:PHE:CE2	1:B:474:ILE:HG21	2.48	0.48
1:C:313:MET:O	1:C:317:PHE:CE1	2.66	0.48
1:A:210:GLN:CG	1:A:249:ILE:HG23	2.43	0.48
1:C:637:ARG:CB	1:C:642:ASN:HB3	2.44	0.48
1:C:889:ALA:HB2	1:C:898:PRO:HG3	1.94	0.48
1:A:597:TYR:C	1:A:597:TYR:CD1	2.86	0.48
1:A:991:ILE:O	1:A:992:SER:CB	2.61	0.48
1:B:913:LEU:O	1:B:917:THR:CB	2.62	0.48
1:C:204:ILE:HG22	1:C:205:THR:N	2.28	0.48
1:C:114:ALA:HA	1:C:117:LEU:HD12	1.95	0.48
1:A:727:PHE:CZ	1:A:807:SER:HB3	2.49	0.48
1:B:616:GLY:HA3	1:B:624:THR:HG22	1.95	0.48
1:B:446:ALA:O	1:B:447:MET:C	2.52	0.48
1:C:577:GLN:HA	1:C:624:THR:HA	1.96	0.48
1:B:111:LEU:HD22	1:B:129:VAL:HG23	1.96	0.48
1:B:55:LYS:CE	1:B:59:ASP:OD1	2.61	0.48
1:C:188:MET:HA	1:C:266:ALA:HB2	1.96	0.48
1:C:586:ARG:O	1:C:590:VAL:HG23	2.14	0.48
1:A:471:SER:O	1:A:475:VAL:CG1	2.59	0.48
1:B:717:ARG:N	1:B:717:ARG:CD	2.77	0.48
1:C:395:MET:C	1:C:397:GLY:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HB3	1:A:426:PRO:HD2	1.95	0.48
1:A:194:ASN:ND2	1:A:790:TYR:CD2	2.82	0.48
1:A:733:GLN:HE22	1:A:743:ILE:HD12	1.78	0.48
1:A:238:THR:OG1	1:A:239:ARG:N	2.47	0.48
1:A:527:TYR:HE2	1:A:972:LEU:HG	1.78	0.48
1:B:600:THR:C	1:B:602:GLU:H	2.17	0.48
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.44	0.48
1:C:527:TYR:CZ	1:C:1019:ILE:HG13	2.49	0.48
1:B:524:THR:O	1:B:528:THR:N	2.40	0.48
1:B:364:ALA:HB2	1:B:497:LEU:HG	1.94	0.48
1:C:367:ILE:HD13	1:C:492:LEU:HD22	1.95	0.48
1:C:655:PHE:HB3	1:C:663:VAL:HG23	1.95	0.48
1:B:306:ILE:HG23	1:B:310:LEU:HD12	1.96	0.48
1:A:896:SER:OG	1:A:897:ILE:N	2.47	0.48
1:B:940:LYS:HA	1:B:943:ILE:HG22	1.95	0.48
1:B:188:MET:HB3	1:B:789:TRP:HH2	1.79	0.48
1:A:367:ILE:HA	1:A:370:ILE:HG22	1.96	0.48
1:B:518:ARG:HA	1:B:521:GLU:CD	2.34	0.48
1:B:640:GLU:H	1:B:643:LYS:HG2	1.79	0.48
1:B:452:VAL:HG11	1:B:932:LEU:O	2.14	0.47
1:C:33:ALA:HA	1:C:300:LEU:HD12	1.96	0.47
1:B:144:ASN:HD21	1:B:148:THR:N	2.10	0.47
1:B:372:VAL:HG13	1:B:405:LEU:HD21	1.96	0.47
1:C:824:SER:OG	1:C:825:MET:N	2.47	0.47
1:C:982:PHE:O	1:C:984:LEU:N	2.47	0.47
1:C:223:PRO:HA	1:C:224:PRO:HD3	1.75	0.47
1:C:901:VAL:O	1:C:904:VAL:HG23	2.14	0.47
1:A:901:VAL:HA	1:A:942:ALA:HB1	1.97	0.47
1:C:894:SER:HG	1:C:897:ILE:HG12	1.76	0.47
1:A:449:LEU:O	1:A:453:PHE:HD1	1.97	0.47
1:A:911:GLY:HA2	1:A:914:LEU:HB2	1.96	0.47
1:A:685:ILE:HG22	1:A:686:ASP:N	2.29	0.47
1:A:550:VAL:O	1:A:551:GLY:C	2.53	0.47
1:B:688:ALA:O	1:B:690:LEU:N	2.46	0.47
1:A:964:THR:HG21	1:A:1027:VAL:HG23	1.96	0.47
1:B:350:LEU:O	1:B:984:LEU:HB3	2.13	0.47
1:A:72:ILE:HD13	1:A:107:VAL:HA	1.95	0.47
1:B:713:LEU:HD13	1:B:843:LEU:HD13	1.95	0.47
1:C:317:PHE:CD2	1:C:321:LEU:HD12	2.49	0.47
1:B:143:ILE:CD1	1:B:285:PRO:O	2.60	0.47
1:C:291:ILE:HD13	1:C:306:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:LEU:HD11	1:B:1028:VAL:HG21	1.95	0.47
1:A:189:ASN:ND2	1:A:779:TYR:OH	2.47	0.47
1:B:762:PHE:C	1:B:763:ILE:HD12	2.34	0.47
1:B:372:VAL:HB	1:B:373:PRO:CD	2.40	0.47
1:A:211:ASN:HB3	1:A:760:ASN:HD21	1.80	0.47
1:C:633:ASP:O	1:C:634:TRP:HB2	2.14	0.47
1:C:453:PHE:C	1:C:455:PRO:HD2	2.34	0.47
1:C:594:VAL:HG13	1:C:598:TYR:CE1	2.48	0.47
1:B:650:ARG:O	1:B:654:ALA:N	2.44	0.47
1:A:112:GLN:HE22	1:C:112:GLN:HG2	1.80	0.47
1:B:578:LEU:HD23	1:B:578:LEU:N	2.29	0.47
1:C:431:THR:O	1:C:434:SER:HB2	2.14	0.47
1:B:463:THR:HA	1:B:466:ILE:HD12	1.97	0.47
1:B:843:LEU:HD23	1:B:847:LEU:HG	1.96	0.47
1:B:335:ILE:O	1:B:336:SER:C	2.53	0.47
1:C:933:THR:O	1:C:937:LEU:HB2	2.14	0.47
1:C:34:GLN:NE2	1:C:299:ALA:HB3	2.11	0.47
1:C:62:THR:OG1	1:C:88:VAL:HG13	2.14	0.47
1:B:631:LEU:HB3	1:B:637:ARG:NH1	2.19	0.47
1:A:901:VAL:HG13	1:A:942:ALA:HB3	1.97	0.47
1:B:866:GLU:O	1:B:867:ARG:C	2.52	0.47
1:B:225:VAL:O	1:B:226:LYS:C	2.52	0.47
1:A:1021:PHE:CD1	1:A:1025:PHE:HE1	2.32	0.47
1:B:68:ASN:C	1:B:70:ASN:N	2.65	0.47
1:A:250:LEU:CD2	1:A:259:ARG:HD2	2.45	0.47
1:B:805:SER:OG	1:B:806:SER:N	2.47	0.47
1:C:18:ILE:O	1:C:19:ILE:C	2.53	0.47
1:A:542:LEU:HD23	1:A:1028:VAL:HG21	1.96	0.47
1:C:4:PHE:O	1:C:8:ARG:NH1	2.48	0.47
1:A:198:LEU:HD22	1:A:202:ASP:HB3	1.96	0.47
1:A:69:MET:CE	1:A:107:VAL:HG13	2.44	0.47
1:B:1022:VAL:HG23	1:B:1023:PRO:CD	2.44	0.47
1:A:726:GLN:NE2	1:C:235:ILE:HG13	2.30	0.47
1:A:961:ILE:O	1:A:965:LEU:HD23	2.15	0.47
1:B:314:GLU:N	1:B:315:PRO:CD	2.77	0.47
1:C:655:PHE:O	1:C:657:GLN:N	2.48	0.47
1:C:881:LEU:C	1:C:883:VAL:H	2.18	0.47
1:A:655:PHE:O	1:A:657:GLN:N	2.43	0.47
1:A:636:ASP:OD2	1:A:636:ASP:N	2.48	0.47
1:B:490:PRO:O	1:B:493:CYS:N	2.48	0.47
1:B:45:ILE:HD13	1:B:65:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ILE:HD12	1:B:940:LYS:CG	2.44	0.47
1:C:958:LYS:HB3	1:C:962:GLU:HB2	1.96	0.47
1:B:592:ASN:HA	1:B:595:THR:CG2	2.45	0.47
1:A:780:ARG:O	1:A:780:ARG:HD2	2.14	0.47
1:C:882:ILE:O	1:C:882:ILE:CG2	2.63	0.47
1:C:395:MET:C	1:C:397:GLY:N	2.69	0.47
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.95	0.47
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.96	0.47
1:A:516:PHE:CG	1:A:517:ASN:N	2.82	0.47
1:A:108:GLN:HG3	1:B:112:GLN:OE1	2.15	0.47
1:A:671:ILE:HG13	1:A:674:LEU:CB	2.45	0.47
1:C:466:ILE:HG13	1:C:563:PHE:CZ	2.50	0.47
1:C:3:ASN:C	1:C:5:PHE:N	2.68	0.47
1:C:615:PHE:HE2	2:C:3402:ERY:H341	1.80	0.47
1:C:912:ALA:HB1	1:C:927:PHE:CE1	2.50	0.47
1:C:353:LEU:O	1:C:355:MET:N	2.48	0.47
1:C:120:GLN:O	1:C:124:GLN:HG2	2.15	0.46
1:B:356:TYR:O	1:B:358:PHE:N	2.35	0.46
1:A:609:VAL:HG23	1:A:609:VAL:O	2.15	0.46
1:B:1031:ARG:HD2	1:B:1035:ARG:HH21	1.80	0.46
1:A:104:GLN:OE1	1:A:131:LYS:HG3	2.15	0.46
1:B:452:VAL:O	1:B:453:PHE:CB	2.63	0.46
1:C:34:GLN:HG2	1:C:35:TYR:H	1.79	0.46
1:C:146:ASP:C	1:C:148:THR:N	2.68	0.46
1:B:23:GLY:H	1:B:381:ALA:HB2	1.79	0.46
1:B:671:ILE:HB	1:B:672:VAL:H	1.50	0.46
1:A:41:PRO:HD3	1:A:96:SER:O	2.15	0.46
1:B:326:PRO:HB3	1:B:610:PHE:HB2	1.97	0.46
1:B:194:ASN:HB2	1:B:790:TYR:HB2	1.96	0.46
1:B:681:ASP:CB	1:B:860:THR:CG2	2.93	0.46
1:B:937:LEU:O	1:B:940:LYS:HB3	2.16	0.46
1:B:356:TYR:O	1:B:360:GLN:HG2	2.15	0.46
1:A:376:LEU:O	1:A:378:GLY:N	2.39	0.46
1:B:200:PRO:HA	1:B:203:VAL:HG23	1.97	0.46
1:B:848:ALA:O	1:B:850:LYS:N	2.39	0.46
1:A:261:LEU:HD13	1:A:263:ARG:HH11	1.79	0.46
1:B:669:PRO:HB2	1:B:862:MET:SD	2.55	0.46
1:C:635:ALA:C	1:C:637:ARG:H	2.18	0.46
1:B:213:GLN:CB	1:B:239:ARG:HD2	2.43	0.46
1:B:121:GLU:HG2	1:B:121:GLU:H	1.59	0.46
1:B:69:MET:HB3	1:B:92:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:ALA:HB1	1:C:11:PHE:HA	1.97	0.46
1:C:578:LEU:HD22	1:C:661:ALA:HB2	1.97	0.46
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.50	0.46
1:A:231:ASN:CB	1:B:622:GLN:HE22	2.28	0.46
1:C:912:ALA:HB1	1:C:927:PHE:HE1	1.80	0.46
1:A:456:MET:C	1:A:458:PHE:H	2.15	0.46
1:C:743:ILE:HA	1:C:746:ILE:HD12	1.97	0.46
1:C:477:ALA:C	1:C:479:ALA:H	2.18	0.46
1:A:316:PHE:HD2	1:A:316:PHE:N	2.14	0.46
1:B:408:ASP:OD2	1:B:445:ILE:HB	2.16	0.46
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.51	0.46
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.98	0.46
1:B:416:VAL:HG22	1:B:431:THR:HA	1.96	0.46
1:C:527:TYR:CE2	1:C:968:VAL:O	2.67	0.46
1:A:1022:VAL:HA	1:A:1025:PHE:CD1	2.50	0.46
1:A:391:ASN:O	1:A:392:THR:C	2.54	0.46
1:C:563:PHE:CE2	1:C:564:LEU:HD12	2.51	0.46
1:A:249:ILE:HB	1:A:262:LEU:HB2	1.98	0.46
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.97	0.46
1:B:833:PRO:C	1:B:835:LYS:H	2.18	0.46
1:B:729:ILE:CG1	1:B:730:ASP:N	2.79	0.46
1:B:398:MET:HG3	1:B:473:THR:CG2	2.46	0.46
1:A:527:TYR:C	1:A:529:ASP:H	2.17	0.46
1:B:183:ALA:CB	1:B:273:GLU:HB3	2.45	0.46
1:A:652:THR:HB	1:A:653:ARG:HH21	1.81	0.46
1:A:426:PRO:CB	1:A:427:PRO:CD	2.94	0.46
1:A:444:GLY:HA3	1:A:891:LEU:HD22	1.97	0.46
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.98	0.46
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.51	0.46
1:C:49:TYR:N	1:C:122:VAL:HG23	2.31	0.46
1:B:45:ILE:HG12	1:B:129:VAL:HG22	1.97	0.46
1:A:240:LEU:N	1:A:240:LEU:CD1	2.79	0.46
1:B:671:ILE:C	1:B:673:GLU:N	2.69	0.46
1:C:1016:VAL:O	1:C:1018:ALA:N	2.42	0.46
1:C:683:GLU:HG3	1:C:819:TYR:CD2	2.51	0.46
1:C:111:LEU:HD13	1:C:115:MET:HE3	1.97	0.46
1:C:947:GLU:C	1:C:949:ALA:N	2.68	0.46
1:C:346:GLU:O	1:C:350:LEU:HB2	2.16	0.46
1:C:951:ASP:C	1:C:953:MET:H	2.19	0.46
1:A:575:MET:CE	1:A:577:GLN:HE21	2.29	0.46
1:B:919:ARG:NH2	1:B:990:VAL:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:ASN:HA	1:C:595:THR:OG1	2.16	0.46
1:B:833:PRO:O	1:B:835:LYS:N	2.49	0.46
1:B:13:TRP:CD1	1:C:895:TRP:HZ2	2.33	0.46
1:C:164:ASP:O	1:C:167:SER:HB2	2.16	0.46
1:C:102:ILE:O	1:C:105:VAL:N	2.49	0.46
1:B:84:SER:HB3	1:B:814:PRO:HA	1.98	0.46
1:B:151:GLN:NE2	1:B:279:ALA:H	2.14	0.46
1:A:671:ILE:HG13	1:A:674:LEU:HB3	1.96	0.46
1:B:36:PRO:HD3	1:B:391:ASN:HD21	1.77	0.46
1:C:912:ALA:C	1:C:914:LEU:N	2.69	0.46
1:C:220:GLY:H	1:C:231:ASN:HD22	1.64	0.46
1:C:348:ILE:HG13	1:C:349:ILE:N	2.31	0.46
1:B:418:ARG:HB3	1:B:418:ARG:NH1	2.31	0.46
1:A:317:PHE:HB3	1:A:321:LEU:CB	2.26	0.45
1:A:354:VAL:O	1:A:356:TYR:N	2.48	0.45
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.98	0.45
1:B:464:GLY:O	1:B:468:ARG:HD3	2.16	0.45
1:C:357:LEU:HD23	1:C:358:PHE:CE2	2.51	0.45
1:C:973:ARG:HG2	1:C:977:MET:HE3	1.97	0.45
1:C:367:ILE:HG21	1:C:497:LEU:HD23	1.98	0.45
1:B:414:GLU:OE2	1:B:974:PRO:HD3	2.16	0.45
1:B:602:GLU:C	1:B:604:ASN:H	2.18	0.45
1:A:391:ASN:H	1:A:394:THR:HG22	1.80	0.45
1:B:935:ILE:O	1:B:935:ILE:HG22	2.17	0.45
1:C:54:ALA:HB2	1:C:84:SER:CA	2.46	0.45
1:C:3:ASN:O	1:C:5:PHE:N	2.45	0.45
1:A:228:GLN:O	1:B:583:THR:HG21	2.16	0.45
1:B:197:GLN:O	1:B:792:ARG:NH2	2.50	0.45
1:B:356:TYR:C	1:B:358:PHE:H	2.17	0.45
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.41	0.45
1:C:898:PRO:HG2	1:C:899:PHE:CD1	2.51	0.45
1:B:349:ILE:C	1:B:351:VAL:N	2.69	0.45
1:B:984:LEU:HA	1:B:987:MET:HB2	1.97	0.45
1:C:91:THR:HG21	2:C:3402:ERY:H272	1.98	0.45
1:A:682:PHE:HE2	1:A:684:LEU:HD12	1.82	0.45
1:A:95:GLU:O	1:A:96:SER:C	2.55	0.45
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.95	0.45
1:C:330:THR:N	1:C:331:PRO:CD	2.79	0.45
1:B:843:LEU:HD23	1:B:847:LEU:CD2	2.46	0.45
1:A:189:ASN:ND2	1:A:779:TYR:CZ	2.84	0.45
1:B:427:PRO:C	1:B:429:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:VAL:O	1:C:33:ALA:C	2.54	0.45
1:C:373:PRO:O	1:C:377:LEU:HB2	2.15	0.45
1:C:733:GLN:HA	1:C:733:GLN:OE1	2.16	0.45
1:B:15:ILE:O	1:B:19:ILE:HG12	2.17	0.45
1:C:351:VAL:HG13	1:C:369:THR:HG22	1.99	0.45
1:A:307:ARG:NH2	1:A:328:ASP:OD2	2.49	0.45
1:A:974:PRO:C	1:A:976:LEU:H	2.18	0.45
1:A:447:MET:CB	1:A:887:CYS:SG	2.91	0.45
1:C:408:ASP:OD2	1:C:940:LYS:NZ	2.46	0.45
1:A:199:THR:HG22	1:A:791:VAL:HA	1.96	0.45
1:C:176:GLN:HE21	1:C:620:ARG:NH1	2.11	0.45
1:B:198:LEU:HD23	1:B:792:ARG:HH22	1.81	0.45
1:A:786:ILE:O	1:A:787:GLY:C	2.54	0.45
2:C:3402:ERY:H343	2:C:3402:ERY:H353	1.98	0.45
1:C:1015:THR:O	1:C:1019:ILE:HB	2.17	0.45
1:C:801:PHE:CD1	1:C:804:PHE:HE1	2.35	0.45
1:B:639:GLY:HA2	1:B:643:LYS:NZ	2.31	0.45
1:A:714:THR:H	1:A:832:ALA:HB2	1.80	0.45
1:C:54:ALA:HB2	1:C:84:SER:CB	2.46	0.45
1:A:239:ARG:CD	1:A:763:ILE:HG13	2.47	0.45
1:C:937:LEU:HD12	1:C:937:LEU:HA	1.88	0.45
1:C:6:ILE:O	1:C:9:PRO:HD3	2.16	0.45
1:A:901:VAL:HG13	1:A:942:ALA:CB	2.46	0.45
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.52	0.45
1:C:251:LEU:CD1	1:C:262:LEU:HA	2.47	0.45
1:A:216:ALA:O	1:A:217:GLY:O	2.35	0.45
1:B:414:GLU:CD	1:B:974:PRO:HG3	2.37	0.45
1:A:800:PRO:O	1:A:803:ALA:HB3	2.17	0.45
1:A:909:VAL:O	1:A:913:LEU:HD23	2.17	0.45
1:B:327:TYR:O	1:B:327:TYR:CG	2.70	0.45
1:C:27:ILE:HD11	1:C:380:PHE:CE2	2.52	0.45
1:C:463:THR:HA	1:C:466:ILE:CG1	2.46	0.45
1:B:934:THR:HA	1:B:937:LEU:HB2	1.98	0.45
1:B:409:ALA:HA	1:B:485:ALA:CB	2.47	0.45
1:A:489:THR:HG22	1:A:490:PRO:HD3	1.98	0.45
1:C:527:TYR:C	1:C:529:ASP:H	2.19	0.45
1:A:96:SER:OG	1:A:97:GLY:N	2.48	0.45
1:A:180:SER:O	1:A:181:GLN:CB	2.63	0.45
1:C:734:GLU:HA	1:C:737:GLN:CG	2.46	0.45
1:C:986:VAL:CG1	1:C:986:VAL:O	2.64	0.45
1:C:801:PHE:O	1:C:803:ALA:N	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:HD11	1:B:490:PRO:HB2	1.98	0.45
1:B:967:ALA:C	1:B:969:ARG:N	2.68	0.45
1:C:314:GLU:N	1:C:315:PRO:HD2	2.32	0.45
1:B:892:TYR:OH	1:B:947:GLU:HB2	2.17	0.45
1:B:27:ILE:HG22	1:B:380:PHE:CD2	2.51	0.45
1:B:399:VAL:O	1:B:402:ILE:CG2	2.59	0.45
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.16	0.45
1:C:474:ILE:HG22	1:C:475:VAL:N	2.30	0.45
1:B:57:VAL:HG12	1:B:82:SER:HB2	1.98	0.45
1:A:240:LEU:H	1:A:240:LEU:CD1	2.30	0.45
1:C:176:GLN:NE2	1:C:620:ARG:HH12	2.09	0.45
1:C:672:VAL:HG13	1:C:673:GLU:H	1.77	0.45
1:B:343:THR:HA	1:B:346:GLU:HG2	1.99	0.45
1:B:232:ALA:HB1	1:C:725:PRO:O	2.17	0.45
1:A:200:PRO:HG2	1:A:749:THR:HG23	1.98	0.45
1:B:306:ILE:CG2	1:B:310:LEU:HD12	2.47	0.45
1:A:250:LEU:HD23	1:A:259:ARG:HD2	1.99	0.45
1:A:949:ALA:O	1:A:953:MET:HB2	2.16	0.45
1:A:735:LYS:O	1:A:739:LEU:HD22	2.15	0.45
1:B:177:LEU:HD12	1:B:288:GLY:O	2.17	0.45
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.52	0.45
1:B:484:VAL:HG12	1:B:489:THR:OG1	2.16	0.45
1:A:61:VAL:HG21	1:A:122:VAL:HG21	1.98	0.45
1:B:356:TYR:O	1:B:360:GLN:N	2.50	0.45
1:B:358:PHE:CD1	1:B:977:MET:HB3	2.51	0.45
1:B:564:LEU:HG	1:B:925:VAL:HG11	1.98	0.45
1:B:420:MET:SD	1:B:425:LEU:HA	2.57	0.45
1:B:525:HIS:HA	1:B:528:THR:CG2	2.47	0.45
1:B:967:ALA:C	1:B:969:ARG:H	2.20	0.45
1:C:528:THR:CG2	1:C:969:ARG:HG3	2.47	0.45
1:C:838:GLY:O	1:C:842:GLU:HB2	2.17	0.44
1:A:367:ILE:CG1	1:A:368:PRO:HD3	2.46	0.44
1:B:230:LEU:HD21	1:C:809:TRP:CH2	2.53	0.44
1:B:204:ILE:O	1:B:205:THR:C	2.55	0.44
1:A:66:GLU:OE2	1:A:821:GLY:HA2	2.17	0.44
1:A:197:GLN:HA	1:A:798:MET:SD	2.57	0.44
1:A:18:ILE:O	1:A:19:ILE:C	2.54	0.44
1:C:684:LEU:HD21	1:C:699:ARG:HA	1.99	0.44
1:C:653:ARG:HG3	1:C:654:ALA:N	2.32	0.44
1:B:111:LEU:O	1:B:113:LEU:N	2.51	0.44
1:B:57:VAL:HG12	1:B:58:GLN:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:CG1	1:C:88:VAL:HG22	2.46	0.44
1:C:452:VAL:HG11	1:C:935:ILE:HG23	1.98	0.44
1:B:919:ARG:HG3	1:B:920:GLY:H	1.82	0.44
1:C:767:ARG:CG	1:C:767:ARG:NH1	2.77	0.44
1:C:69:MET:CG	1:C:92:LEU:HD21	2.47	0.44
1:B:717:ARG:HD3	1:B:717:ARG:N	2.31	0.44
1:B:680:PHE:CD1	1:B:859:TRP:CZ3	3.05	0.44
1:C:367:ILE:CD1	1:C:492:LEU:HD22	2.48	0.44
1:B:712:MET:HA	1:B:834:GLY:CA	2.47	0.44
1:C:350:LEU:O	1:C:350:LEU:HD23	2.17	0.44
1:A:165:ALA:O	1:A:169:THR:HG23	2.17	0.44
1:C:145:THR:C	1:C:147:GLY:H	2.19	0.44
1:C:5:PHE:HD2	1:C:12:ALA:HB2	1.81	0.44
1:B:343:THR:O	1:B:347:ALA:HB2	2.17	0.44
1:C:44:THR:HB	1:C:91:THR:HB	1.99	0.44
1:A:355:MET:HB3	1:A:365:THR:HG22	2.00	0.44
1:C:191:ASN:O	1:C:194:ASN:N	2.48	0.44
1:B:696:THR:HG23	1:B:825:MET:HE1	1.99	0.44
1:C:428:LYS:HG2	1:C:428:LYS:O	2.17	0.44
1:C:467:TYR:OH	1:C:925:VAL:HG12	2.17	0.44
1:B:34:GLN:OE1	1:B:35:TYR:CD1	2.71	0.44
1:B:35:TYR:HB3	1:B:38:ILE:HG13	1.99	0.44
1:A:207:ILE:CB	1:A:759:VAL:HG11	2.46	0.44
1:C:686:ASP:CG	1:C:690:LEU:HB2	2.38	0.44
1:C:330:THR:N	1:C:331:PRO:HD2	2.33	0.44
1:C:763:ILE:N	1:C:763:ILE:HD12	2.33	0.44
1:A:415:ASN:O	1:A:434:SER:HB2	2.17	0.44
1:C:410:ILE:O	1:C:411:VAL:C	2.55	0.44
1:B:87:THR:HG21	1:B:620:ARG:CZ	2.47	0.44
1:B:945:ILE:HG13	1:B:946:VAL:HG23	2.00	0.44
1:C:830:GLN:OE1	1:C:832:ALA:HA	2.18	0.44
1:A:552:MET:HB2	1:A:910:ILE:HG23	1.99	0.44
1:C:72:ILE:HB	1:C:75:LEU:HD12	2.00	0.44
1:C:544:LEU:O	1:C:548:ILE:HG13	2.17	0.44
1:C:912:ALA:N	1:C:1010:GLY:HA2	2.33	0.44
1:C:1030:ARG:C	1:C:1032:ARG:H	2.21	0.44
1:B:768:VAL:HG23	1:C:63:GLN:CD	2.38	0.44
1:B:972:LEU:N	1:B:974:PRO:HD2	2.32	0.44
1:A:324:VAL:HG12	1:A:325:TYR:N	2.33	0.44
1:A:930:GLY:C	1:A:932:LEU:H	2.21	0.44
1:A:879:ILE:O	1:A:883:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:LEU:HA	1:C:452:VAL:HG23	2.00	0.44
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.99	0.44
1:A:942:ALA:O	1:A:946:VAL:HB	2.17	0.44
1:A:355:MET:HG2	1:A:365:THR:HA	1.99	0.44
1:C:115:MET:HA	1:C:115:MET:HE2	1.98	0.44
1:A:583:THR:O	1:A:587:THR:N	2.49	0.44
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.98	0.44
1:C:255:GLN:C	1:C:257:GLY:N	2.71	0.44
1:C:919:ARG:HG2	1:C:1005:THR:HG21	1.99	0.44
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.99	0.44
1:A:682:PHE:HB2	1:A:859:TRP:CZ3	2.52	0.44
1:B:859:TRP:HB3	1:B:863:SER:HB3	2.00	0.44
1:C:228:GLN:NE2	1:C:229:GLN:O	2.37	0.44
1:A:124:GLN:HG2	1:A:758:TYR:HE2	1.81	0.44
1:A:45:ILE:HD11	1:A:92:LEU:HD11	2.00	0.44
1:C:68:ASN:O	1:C:70:ASN:N	2.51	0.44
1:B:897:ILE:O	1:B:901:VAL:HG23	2.18	0.44
1:C:467:TYR:O	1:C:470:PHE:N	2.51	0.44
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.53	0.44
1:A:750:LEU:HD13	1:C:216:ALA:HB1	1.99	0.44
1:A:576:VAL:HG11	1:A:591:LEU:HD23	1.99	0.44
1:B:455:PRO:HG3	1:B:880:SER:HA	1.99	0.44
1:A:773:VAL:CG1	1:A:773:VAL:O	2.66	0.44
1:C:684:LEU:HD22	1:C:702:LEU:HD23	2.00	0.44
1:C:866:GLU:C	1:C:867:ARG:HG2	2.38	0.44
1:C:885:PHE:O	1:C:885:PHE:CG	2.70	0.44
1:C:564:LEU:HD13	1:C:671:ILE:HB	2.00	0.44
1:C:210:GLN:HB2	1:C:249:ILE:HD12	1.99	0.44
1:C:896:SER:C	1:C:898:PRO:HD2	2.38	0.44
2:C:3402:ERY:H321	2:C:3402:ERY:H8	1.78	0.44
1:A:375:VAL:O	1:A:379:THR:N	2.51	0.44
1:A:583:THR:HG22	1:A:585:GLU:H	1.82	0.44
1:A:634:TRP:CZ3	1:A:995:ALA:HA	2.52	0.44
1:C:953:MET:HG3	1:C:963:ALA:HB2	2.00	0.44
1:A:894:SER:C	1:A:896:SER:H	2.20	0.44
1:B:151:GLN:O	1:B:153:ASP:N	2.43	0.44
1:B:111:LEU:HD22	1:B:129:VAL:HG21	1.99	0.43
1:B:574:THR:HA	1:B:665:ALA:HA	1.98	0.43
1:C:897:ILE:N	1:C:898:PRO:CD	2.80	0.43
1:B:560:PRO:CB	1:B:836:SER:HB2	2.42	0.43
1:C:332:PHE:O	1:C:336:SER:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:MET:HE2	1:C:228:GLN:OE1	2.17	0.43
1:B:843:LEU:O	1:B:847:LEU:HD23	2.18	0.43
1:B:754:TRP:CH2	1:B:785:ASP:HB2	2.53	0.43
1:A:515:TRP:O	1:A:516:PHE:HB2	2.18	0.43
1:A:993:THR:HG21	1:A:1000:GLN:OE1	2.18	0.43
1:C:181:GLN:HG2	1:C:769:LYS:HE2	2.00	0.43
1:B:950:LYS:O	1:B:954:ASP:HB3	2.18	0.43
1:C:395:MET:O	1:C:397:GLY:N	2.51	0.43
1:B:704:ALA:O	1:B:705:GLU:HB3	2.17	0.43
1:A:635:ALA:C	1:A:637:ARG:H	2.22	0.43
1:B:26:ALA:HB1	1:B:384:ALA:HB2	2.00	0.43
1:A:886:LEU:HD11	1:C:17:ILE:HB	1.99	0.43
1:A:193:LEU:HD21	1:A:199:THR:HA	2.00	0.43
1:B:262:LEU:O	1:B:265:VAL:N	2.51	0.43
1:B:355:MET:SD	1:B:369:THR:HG23	2.58	0.43
1:B:419:VAL:O	1:B:419:VAL:CG1	2.65	0.43
1:C:137:LEU:HD12	1:C:138:MET:HB3	2.01	0.43
1:C:191:ASN:O	1:C:192:GLU:C	2.56	0.43
1:C:824:SER:O	1:C:825:MET:HB2	2.18	0.43
1:B:293:LEU:HD22	1:B:294:ALA:N	2.33	0.43
1:B:367:ILE:N	1:B:368:PRO:HD2	2.33	0.43
1:A:367:ILE:CD1	1:A:368:PRO:HD3	2.48	0.43
1:A:682:PHE:HD1	1:A:859:TRP:CH2	2.36	0.43
1:A:966:ASP:HA	1:A:969:ARG:HD2	1.99	0.43
1:B:25:LEU:O	1:B:28:LEU:HG	2.18	0.43
1:C:353:LEU:C	1:C:355:MET:N	2.72	0.43
1:C:208:LYS:HA	1:C:760:ASN:ND2	2.32	0.43
1:C:314:GLU:N	1:C:315:PRO:CD	2.82	0.43
1:C:80:SER:HA	1:C:90:ILE:HA	2.00	0.43
1:C:983:ILE:HD11	1:C:1011:MET:HG2	2.00	0.43
1:C:674:LEU:HD11	1:C:865:GLN:HB2	2.01	0.43
1:C:72:ILE:HG22	1:C:94:PHE:HE2	1.83	0.43
1:B:298:ASN:ND2	1:B:298:ASN:O	2.49	0.43
1:A:535:LEU:HB3	1:A:961:ILE:HD12	2.00	0.43
1:B:699:ARG:HB3	1:B:699:ARG:NH1	2.33	0.43
1:A:699:ARG:NH2	1:A:722:GLU:OE2	2.49	0.43
1:B:901:VAL:HG22	1:B:1026:PHE:HZ	1.84	0.43
1:B:349:ILE:HG22	1:B:350:LEU:HD23	2.00	0.43
1:A:72:ILE:HG23	1:A:106:GLN:HB3	1.99	0.43
1:A:186:ILE:O	1:A:186:ILE:HG22	2.18	0.43
1:A:225:VAL:O	1:A:226:LYS:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:MET:O	1:A:971:ARG:HB2	2.19	0.43
1:C:162:MET:HG2	1:C:313:MET:SD	2.59	0.43
1:A:886:LEU:HD21	1:C:17:ILE:HG21	2.01	0.43
1:B:242:SER:C	1:B:244:GLU:N	2.72	0.43
1:B:393:LEU:CB	1:B:469:GLN:HG2	2.49	0.43
1:B:964:THR:HG22	1:B:1023:PRO:HB3	2.01	0.43
1:A:219:LEU:H	1:A:231:ASN:ND2	2.17	0.43
1:C:214:VAL:HG23	1:C:236:ALA:HB3	2.00	0.43
1:B:651:ALA:HB1	1:B:655:PHE:CE2	2.53	0.43
1:C:77:TYR:CD2	1:C:77:TYR:N	2.87	0.43
1:C:244:GLU:O	1:C:263:ARG:NH2	2.52	0.43
1:C:34:GLN:CG	1:C:35:TYR:H	2.32	0.43
1:C:713:LEU:HD13	1:C:713:LEU:N	2.33	0.43
1:B:24:GLY:CA	1:B:27:ILE:HG23	2.48	0.43
1:B:778:LYS:C	1:B:780:ARG:H	2.22	0.43
1:C:124:GLN:HB2	1:C:758:TYR:CE2	2.47	0.43
1:C:189:ASN:HA	1:C:190:PRO:HD3	1.84	0.43
1:B:219:LEU:HD12	1:B:234:ILE:HD11	2.00	0.43
1:B:967:ALA:O	1:B:969:ARG:N	2.52	0.43
1:B:961:ILE:O	1:B:965:LEU:HD23	2.18	0.43
1:A:997:SER:HB2	1:A:998:GLY:H	1.62	0.43
1:C:199:THR:OG1	1:C:201:VAL:N	2.51	0.43
1:B:448:VAL:HG21	1:B:888:LEU:HD21	2.01	0.43
1:B:453:PHE:HA	1:B:456:MET:SD	2.59	0.43
1:B:946:VAL:C	1:B:948:PHE:H	2.22	0.43
1:A:405:LEU:HD23	1:A:477:ALA:HB1	1.99	0.43
1:B:1014:ALA:O	1:B:1018:ALA:HB2	2.19	0.43
1:B:566:ASP:O	1:B:567:GLU:HG2	2.18	0.43
1:B:949:ALA:HB3	1:B:1030:ARG:HH22	1.84	0.43
1:C:605:ASN:CB	1:C:637:ARG:HD3	2.42	0.43
1:B:226:LYS:HA	1:B:226:LYS:NZ	2.33	0.43
1:C:1030:ARG:HB3	1:C:1030:ARG:HE	1.52	0.43
1:C:941:ASN:HD22	1:C:941:ASN:C	2.23	0.43
1:A:584:GLN:H	1:A:622:GLN:HE21	1.66	0.43
1:A:199:THR:HG21	1:A:791:VAL:HA	2.00	0.42
1:C:637:ARG:HB3	1:C:642:ASN:CB	2.48	0.42
1:B:562:SER:O	1:B:924:ASP:HA	2.19	0.42
1:B:240:LEU:HB3	1:B:245:GLU:HB2	2.00	0.42
1:A:457:ALA:O	1:A:458:PHE:HD2	2.02	0.42
1:A:189:ASN:HB3	1:A:192:GLU:HB2	2.00	0.42
1:B:520:PHE:O	1:B:523:SER:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LYS:HG3	1:B:110:LYS:HZ3	1.72	0.42
1:A:536:ARG:H	1:A:536:ARG:HG2	1.56	0.42
1:A:146:ASP:OD2	1:A:146:ASP:N	2.52	0.42
1:B:43:VAL:N	1:B:92:LEU:O	2.48	0.42
1:C:188:MET:HA	1:C:266:ALA:CB	2.49	0.42
1:A:364:ALA:O	1:A:367:ILE:HG13	2.20	0.42
1:A:298:ASN:C	1:A:300:LEU:H	2.22	0.42
1:A:961:ILE:HD11	1:A:1031:ARG:NH1	2.34	0.42
1:B:612:VAL:HG22	1:B:626:ILE:O	2.19	0.42
1:C:982:PHE:O	1:C:985:GLY:N	2.51	0.42
1:A:876:LEU:HA	1:A:879:ILE:HD12	2.01	0.42
1:A:368:PRO:HA	1:A:371:ALA:HB3	2.00	0.42
1:C:202:ASP:O	1:C:203:VAL:C	2.58	0.42
1:A:105:VAL:HG22	1:B:105:VAL:HG13	2.01	0.42
1:A:894:SER:HB2	1:A:896:SER:OG	2.19	0.42
1:C:596:HIS:O	1:C:597:TYR:C	2.57	0.42
1:A:30:LEU:HD21	1:A:384:ALA:HB2	2.01	0.42
1:A:843:LEU:O	1:A:846:GLN:N	2.51	0.42
1:A:206:ALA:C	1:A:208:LYS:N	2.73	0.42
1:A:35:TYR:CG	1:A:671:ILE:HG22	2.55	0.42
1:B:58:GLN:O	1:B:59:ASP:HB2	2.19	0.42
1:C:9:PRO:C	1:C:11:PHE:H	2.21	0.42
1:C:758:TYR:N	1:C:758:TYR:HD1	2.04	0.42
1:B:122:VAL:O	1:B:125:GLN:HB2	2.18	0.42
1:C:203:VAL:HG12	1:C:207:ILE:HD11	2.02	0.42
1:B:717:ARG:NH1	1:B:717:ARG:CG	2.73	0.42
1:C:643:LYS:O	1:C:647:ILE:HG13	2.20	0.42
1:B:545:TYR:CE1	1:B:1025:PHE:HZ	2.37	0.42
1:A:479:ALA:O	1:A:482:VAL:HG12	2.20	0.42
1:B:53:ASP:HB2	1:B:56:THR:OG1	2.20	0.42
1:A:198:LEU:HD22	1:A:202:ASP:CB	2.50	0.42
1:A:354:VAL:HG12	1:A:355:MET:N	2.27	0.42
1:A:361:ASN:HB2	1:A:364:ALA:HB3	2.02	0.42
1:B:924:ASP:HB3	1:B:926:TYR:N	2.34	0.42
1:C:251:LEU:HD11	1:C:262:LEU:HA	2.01	0.42
1:B:300:LEU:HD21	1:B:334:LYS:HG3	2.01	0.42
1:C:324:VAL:O	1:C:326:PRO:HD2	2.20	0.42
1:B:380:PHE:O	1:B:383:LEU:N	2.53	0.42
1:B:733:GLN:HE22	1:B:743:ILE:CG2	2.32	0.42
1:C:545:TYR:CZ	1:C:1025:PHE:CZ	3.07	0.42
1:B:262:LEU:C	1:B:264:ASP:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:GLN:O	1:B:699:ARG:O	2.38	0.42
1:C:534:ILE:HG13	1:C:534:ILE:H	1.74	0.42
1:C:415:ASN:O	1:C:419:VAL:HG22	2.19	0.42
1:C:144:ASN:ND2	1:C:148:THR:N	2.67	0.42
1:C:905:VAL:HG22	1:C:935:ILE:HD11	2.02	0.42
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.55	0.42
1:B:420:MET:SD	1:B:424:GLY:O	2.78	0.42
1:C:818:ARG:HA	1:C:824:SER:N	2.33	0.42
1:B:852:PRO:HB2	1:B:853:THR:H	1.52	0.42
1:C:379:THR:HB	1:C:398:MET:CE	2.50	0.42
1:B:1025:PHE:HA	1:B:1028:VAL:HG12	2.01	0.42
1:B:452:VAL:HG12	1:B:932:LEU:HG	2.02	0.42
1:C:249:ILE:CG2	1:C:250:LEU:N	2.83	0.42
1:B:733:GLN:HE22	1:B:743:ILE:HG21	1.85	0.42
1:B:986:VAL:HG23	1:B:1008:MET:HB2	2.00	0.42
1:C:615:PHE:C	1:C:615:PHE:HD2	2.21	0.42
1:C:202:ASP:OD2	1:C:792:ARG:NH2	2.52	0.42
1:A:1029:VAL:O	1:A:1030:ARG:CB	2.67	0.42
1:A:282:ASN:HD21	1:A:609:VAL:H	1.68	0.42
1:A:323:ILE:HG12	1:A:325:TYR:HE1	1.85	0.42
1:A:889:ALA:HA	1:A:898:PRO:HG3	2.01	0.42
1:C:178:PHE:HA	1:C:277:ILE:HG21	2.02	0.42
1:B:1004:GLY:O	1:B:1006:GLY:N	2.53	0.42
1:B:876:LEU:HD22	1:B:932:LEU:CD1	2.49	0.42
1:C:142:VAL:CG1	1:C:154:ILE:HG23	2.50	0.42
1:B:20:MET:HG2	1:B:374:VAL:HA	2.02	0.42
1:A:102:ILE:HA	1:A:105:VAL:HG23	2.02	0.42
1:A:978:THR:CG2	1:A:979:SER:N	2.83	0.42
1:A:412:VAL:O	1:A:416:VAL:HG23	2.20	0.42
1:B:150:THR:H	1:B:153:ASP:HB3	1.84	0.42
1:B:647:ILE:HG12	1:B:647:ILE:H	1.65	0.42
1:B:136:PHE:H	1:B:136:PHE:HD1	1.65	0.42
1:B:57:VAL:HG21	1:B:86:GLY:HA2	2.01	0.41
1:A:72:ILE:CD1	1:A:107:VAL:HA	2.50	0.41
1:B:924:ASP:HB3	1:B:926:TYR:H	1.84	0.41
1:C:680:PHE:CD2	1:C:680:PHE:N	2.88	0.41
1:B:268:ILE:HD12	1:B:268:ILE:N	2.34	0.41
1:B:602:GLU:C	1:B:604:ASN:N	2.73	0.41
1:B:151:GLN:HE22	1:B:278:ILE:HA	1.85	0.41
1:A:446:ALA:HB2	1:A:482:VAL:HG21	2.01	0.41
1:C:248:LYS:HA	1:C:261:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:739:LEU:HA	1:C:739:LEU:HD12	1.82	0.41
1:C:34:GLN:HB3	1:C:333:VAL:CG2	2.50	0.41
1:C:615:PHE:CE2	2:C:3402:ERY:H341	2.55	0.41
1:C:83:ASP:HA	1:C:815:ARG:HA	2.02	0.41
1:A:46:SER:HA	1:A:88:VAL:O	2.20	0.41
1:A:304:ALA:O	1:A:307:ARG:N	2.53	0.41
1:A:658:ILE:H	1:A:658:ILE:HG12	1.63	0.41
1:C:247:GLY:HA3	1:C:263:ARG:NE	2.35	0.41
1:B:65:ILE:HD11	1:B:118:LEU:HD21	2.02	0.41
1:B:572:PHE:HE2	1:B:631:LEU:HD21	1.84	0.41
1:A:901:VAL:HG11	1:A:943:ILE:HG13	2.01	0.41
1:B:9:PRO:HD2	1:C:893:GLU:OE1	2.20	0.41
1:B:696:THR:O	1:B:699:ARG:HB3	2.20	0.41
1:B:699:ARG:HG2	1:B:700:ASN:N	2.35	0.41
1:B:602:GLU:OE2	1:B:650:ARG:NH2	2.54	0.41
1:C:310:LEU:O	1:C:313:MET:HG2	2.20	0.41
1:C:9:PRO:O	1:C:10:ILE:HB	2.20	0.41
1:A:943:ILE:O	1:A:947:GLU:HB2	2.20	0.41
1:A:892:TYR:CE1	1:A:947:GLU:OE2	2.73	0.41
1:A:193:LEU:HG	1:A:198:LEU:O	2.20	0.41
1:C:545:TYR:CE1	1:C:1025:PHE:CZ	3.08	0.41
1:C:125:GLN:NE2	1:C:758:TYR:CZ	2.85	0.41
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.56	0.41
1:A:31:PRO:HB2	1:A:389:SER:CB	2.48	0.41
1:B:845:GLU:HG3	1:B:857:TYR:OH	2.19	0.41
1:A:218:GLN:O	1:A:234:ILE:HD11	2.20	0.41
1:A:1015:THR:C	1:A:1017:LEU:H	2.23	0.41
1:B:218:GLN:HB2	1:B:232:ALA:O	2.20	0.41
1:B:1021:PHE:O	1:B:1025:PHE:CD1	2.72	0.41
1:B:785:ASP:O	1:B:786:ILE:C	2.59	0.41
1:B:782:LEU:HD23	1:B:782:LEU:H	1.84	0.41
1:A:347:ALA:HA	1:A:350:LEU:HD23	2.02	0.41
1:C:463:THR:C	1:C:465:ALA:N	2.73	0.41
1:B:355:MET:SD	1:B:368:PRO:HB2	2.60	0.41
1:C:137:LEU:CD1	1:C:138:MET:HB3	2.50	0.41
1:B:14:VAL:HG21	1:C:886:LEU:O	2.21	0.41
1:B:911:GLY:HA3	1:B:1013:THR:CG2	2.49	0.41
1:A:527:TYR:C	1:A:529:ASP:N	2.74	0.41
1:B:219:LEU:HD13	1:B:234:ILE:HG12	2.02	0.41
1:A:417:GLU:OE2	1:A:497:LEU:HD22	2.20	0.41
1:B:65:ILE:HG22	1:B:69:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ASN:O	1:C:299:ALA:C	2.58	0.41
1:B:938:SER:C	1:B:940:LYS:H	2.24	0.41
1:C:30:LEU:CD1	1:C:384:ALA:HB2	2.50	0.41
1:C:144:ASN:CB	1:C:154:ILE:HD11	2.51	0.41
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.36	0.41
1:A:251:LEU:O	1:A:252:LYS:HB2	2.21	0.41
1:C:602:GLU:O	1:C:604:ASN:N	2.54	0.41
1:B:61:VAL:HG23	1:B:118:LEU:HD23	2.03	0.41
1:C:463:THR:HG22	1:C:467:TYR:CD1	2.55	0.41
1:C:413:VAL:HG22	1:C:413:VAL:O	2.20	0.41
1:C:5:PHE:CD2	1:C:12:ALA:HB2	2.55	0.41
1:C:431:THR:O	1:C:435:MET:HG2	2.21	0.41
1:B:420:MET:HG2	1:B:426:PRO:CD	2.50	0.41
1:C:1017:LEU:O	1:C:1017:LEU:HD23	2.21	0.41
1:C:226:LYS:HB3	1:C:227:GLY:H	1.74	0.41
1:A:239:ARG:HD3	1:A:763:ILE:HG13	2.03	0.41
1:C:394:THR:HG22	1:C:395:MET:CE	2.50	0.41
1:B:330:THR:N	1:B:331:PRO:CD	2.84	0.41
1:A:1007:VAL:O	1:A:1008:MET:C	2.59	0.41
1:A:692:HIS:C	1:A:694:LYS:H	2.23	0.41
1:A:674:LEU:HD13	1:A:675:GLY:N	2.36	0.41
1:B:58:GLN:HB2	1:B:82:SER:HB3	2.02	0.41
1:C:404:LEU:HD21	1:C:449:LEU:HD12	2.01	0.41
1:B:189:ASN:HD22	1:B:190:PRO:HD2	1.85	0.41
1:C:672:VAL:CG2	1:C:676:THR:H	2.31	0.41
1:C:423:GLU:HB3	1:C:426:PRO:HG2	2.03	0.41
1:B:851:LEU:N	1:B:852:PRO:HD3	2.35	0.41
1:A:551:GLY:O	1:A:555:LEU:HB2	2.21	0.41
1:B:282:ASN:C	1:B:284:GLN:H	2.23	0.41
1:A:465:ALA:O	1:A:469:GLN:HG2	2.20	0.41
1:B:46:SER:O	1:B:127:VAL:HA	2.20	0.41
1:B:57:VAL:CG1	1:B:82:SER:HB2	2.51	0.41
1:C:719:ASN:O	1:C:721:LEU:N	2.53	0.41
1:A:191:ASN:C	1:A:193:LEU:H	2.23	0.41
1:C:160:ALA:HA	1:C:767:ARG:NE	2.36	0.41
1:B:262:LEU:O	1:B:266:ALA:N	2.44	0.41
1:B:239:ARG:NH2	1:B:761:ASP:HB2	2.36	0.41
1:C:617:PHE:CZ	2:C:3402:ERY:H312	2.55	0.41
1:A:365:THR:O	1:A:368:PRO:HD2	2.21	0.41
1:A:294:ALA:HB3	1:A:297:ALA:CB	2.46	0.41
1:B:298:ASN:O	1:B:299:ALA:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:HD12	1:C:886:LEU:HD13	2.02	0.41
1:C:115:MET:CE	1:C:127:VAL:HG21	2.51	0.41
1:A:781:MET:HE1	1:C:225:VAL:N	2.36	0.41
1:C:687:GLN:HB3	1:C:687:GLN:HE21	1.68	0.41
1:B:186:ILE:HB	1:B:773:VAL:HG23	2.02	0.41
1:C:255:GLN:O	1:C:257:GLY:N	2.54	0.41
1:B:782:LEU:HB2	1:B:783:PRO:HD2	2.03	0.41
1:B:462:SER:N	1:B:865:GLN:OE1	2.37	0.41
1:C:249:ILE:HG22	1:C:250:LEU:N	2.36	0.41
1:B:213:GLN:CG	1:C:56:THR:CG2	2.96	0.41
1:B:200:PRO:HD2	1:B:749:THR:CG2	2.51	0.41
1:C:251:LEU:HB2	1:C:260:VAL:O	2.20	0.41
1:A:231:ASN:OD1	1:B:622:GLN:NE2	2.53	0.41
1:C:961:ILE:O	1:C:961:ILE:HG22	2.20	0.41
1:B:310:LEU:HD22	1:B:323:ILE:HG21	2.03	0.41
1:A:579:PRO:O	1:A:580:ALA:C	2.59	0.41
1:B:52:ALA:HB2	1:B:86:GLY:H	1.74	0.40
1:C:142:VAL:HG13	1:C:321:LEU:HD13	2.03	0.40
1:A:904:VAL:HG12	1:A:938:SER:HB3	2.02	0.40
1:A:353:LEU:C	1:A:354:VAL:O	2.59	0.40
1:C:527:TYR:OH	1:C:968:VAL:CG1	2.69	0.40
1:A:153:ASP:HA	1:A:182:TYR:CE1	2.56	0.40
1:B:701:GLN:HE22	1:B:851:LEU:HB2	1.86	0.40
1:C:655:PHE:HB3	1:C:663:VAL:HG21	2.03	0.40
1:A:538:THR:HG23	1:A:540:ARG:NH2	2.37	0.40
1:A:53:ASP:HA	1:A:84:SER:HA	2.03	0.40
1:A:172:VAL:O	1:A:172:VAL:HG23	2.21	0.40
1:C:184:MET:HE3	1:C:184:MET:HA	2.01	0.40
1:B:377:LEU:O	1:B:380:PHE:HB2	2.21	0.40
1:B:383:LEU:O	1:B:384:ALA:C	2.59	0.40
1:B:193:LEU:HD13	1:B:198:LEU:O	2.21	0.40
1:B:13:TRP:O	1:B:17:ILE:HG12	2.21	0.40
1:A:952:LEU:HD11	1:A:966:ASP:HB3	2.03	0.40
1:B:230:LEU:HD21	1:C:809:TRP:HH2	1.86	0.40
1:B:293:LEU:HD22	1:B:294:ALA:H	1.85	0.40
1:B:644:VAL:HA	1:B:647:ILE:HG13	2.03	0.40
1:C:944:LEU:O	1:C:971:ARG:HD2	2.20	0.40
1:B:115:MET:CE	1:B:127:VAL:HG21	2.50	0.40
1:B:445:ILE:HD12	1:B:940:LYS:HG3	2.01	0.40
1:C:1022:VAL:O	1:C:1022:VAL:HG22	2.21	0.40
1:C:423:GLU:HB3	1:C:426:PRO:CD	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ASP:OD1	1:A:690:LEU:HB2	2.21	0.40
1:A:426:PRO:HB3	1:A:427:PRO:CD	2.51	0.40
1:A:184:MET:HB2	1:A:762:PHE:CE2	2.57	0.40
1:A:375:VAL:HG21	1:A:481:SER:HA	2.03	0.40
1:A:620:ARG:NH1	1:A:620:ARG:CG	2.78	0.40
1:B:158:VAL:HA	1:B:162:MET:HG3	2.00	0.40
1:B:231:ASN:ND2	1:B:232:ALA:N	2.70	0.40
1:A:406:VAL:O	1:A:409:ALA:N	2.51	0.40
1:A:897:ILE:O	1:A:900:SER:OG	2.29	0.40
1:B:443:VAL:O	1:B:447:MET:N	2.54	0.40
1:B:681:ASP:CB	1:B:860:THR:HG23	2.51	0.40
1:C:878:ALA:C	1:C:880:SER:H	2.24	0.40
1:B:897:ILE:HA	1:B:900:SER:OG	2.21	0.40
1:B:935:ILE:HG12	1:B:935:ILE:H	1.58	0.40
1:A:708:LYS:C	1:A:709:HIS:HD2	2.24	0.40
1:A:713:LEU:H	1:A:832:ALA:HB2	1.86	0.40
1:C:33:ALA:HB2	1:C:298:ASN:ND2	2.36	0.40
1:C:343:THR:CG2	1:C:989:LEU:HD13	2.42	0.40
1:B:240:LEU:HD13	1:B:245:GLU:HB3	2.02	0.40
1:B:240:LEU:HD22	1:B:245:GLU:HG2	2.03	0.40
1:B:416:VAL:HG21	1:B:431:THR:HG22	2.03	0.40
1:A:726:GLN:N	1:A:810:GLU:O	2.53	0.40
1:B:459:PHE:HB2	1:B:460:GLY:H	1.59	0.40
1:B:231:ASN:HD22	1:B:232:ALA:N	2.20	0.40
1:A:325:TYR:CD1	1:A:325:TYR:N	2.90	0.40
1:B:150:THR:HG22	1:B:151:GLN:H	1.86	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%)	715 (70%)	198 (19%)	105 (10%)	1	5
1	B	1018/1053 (97%)	694 (68%)	214 (21%)	110 (11%)	0	4
1	C	1018/1053 (97%)	734 (72%)	207 (20%)	77 (8%)	1	10
All	All	3054/3159 (97%)	2143 (70%)	619 (20%)	292 (10%)	1	6

All (292) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	134	SER
1	A	160	ALA
1	A	170	SER
1	A	188	MET
1	A	212	ALA
1	A	256	ASP
1	A	293	LEU
1	A	319	SER
1	A	375	VAL
1	A	426	PRO
1	A	516	PHE
1	A	580	ALA
1	A	601	LYS
1	A	638	PRO
1	A	659	LYS
1	A	661	ALA
1	A	678	THR
1	A	775	SER
1	A	788	ASP
1	A	870	GLY
1	A	958	LYS
1	A	971	ARG
1	A	997	SER
1	A	998	GLY
1	A	1008	MET
1	B	2	PRO
1	B	54	ALA
1	B	69	MET
1	B	262	LEU
1	B	299	ALA
1	B	426	PRO
1	B	538	THR
1	B	580	ALA

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Mol	Chain	Res	Type
1	B	581	GLY
1	B	582	ALA
1	B	633	ASP
1	B	656	SER
1	B	671	ILE
1	B	676	THR
1	B	690	LEU
1	B	691	GLY
1	B	805	SER
1	B	806	SER
1	B	820	ASN
1	B	849	SER
1	B	893	GLU
1	B	918	PHE
1	B	921	LEU
1	B	935	ILE
1	B	1033	PHE
1	C	34	GLN
1	C	152	GLU
1	C	226	LYS
1	C	256	ASP
1	C	266	ALA
1	C	319	SER
1	C	427	PRO
1	C	633	ASP
1	C	673	GLU
1	C	713	LEU
1	C	720	GLY
1	C	806	SER
1	C	825	MET
1	C	832	ALA
1	C	836	SER
1	C	837	THR
1	C	921	LEU
1	C	958	LYS
1	C	965	LEU
1	A	64	VAL
1	A	181	GLN
1	A	213	GLN
1	A	217	GLY
1	A	220	GLY
1	A	221	GLY

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Mol	Chain	Res	Type
1	A	227	GLY
1	A	294	ALA
1	A	318	PRO
1	A	354	VAL
1	A	376	LEU
1	A	457	ALA
1	A	460	GLY
1	A	534	ILE
1	A	599	LEU
1	A	656	SER
1	A	670	ALA
1	A	675	GLY
1	A	784	ASP
1	A	787	GLY
1	A	917	THR
1	A	931	LEU
1	A	969	ARG
1	A	992	SER
1	A	1016	VAL
1	A	1017	LEU
1	A	1030	ARG
1	A	1035	ARG
1	B	22	ALA
1	B	84	SER
1	B	140	VAL
1	B	147	GLY
1	B	226	LYS
1	B	243	THR
1	B	263	ARG
1	B	283	GLY
1	B	358	PHE
1	B	360	GLN
1	B	424	GLY
1	B	453	PHE
1	B	486	LEU
1	B	490	PRO
1	B	558	ARG
1	B	601	LYS
1	B	618	ALA
1	B	638	PRO
1	B	658	ILE
1	B	669	PRO

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Mol	Chain	Res	Type
1	B	672	VAL
1	B	689	GLY
1	B	693	GLU
1	B	834	GLY
1	B	852	PRO
1	B	878	ALA
1	B	953	MET
1	B	1005	THR
1	C	4	PHE
1	C	221	GLY
1	C	285	PRO
1	C	411	VAL
1	C	577	GLN
1	C	601	LYS
1	C	602	GLU
1	C	618	ALA
1	C	733	GLN
1	C	802	SER
1	C	820	ASN
1	C	913	LEU
1	C	946	VAL
1	C	960	LEU
1	C	975	ILE
1	C	983	ILE
1	C	997	SER
1	C	998	GLY
1	C	1017	LEU
1	A	182	TYR
1	A	192	GLU
1	A	295	THR
1	A	374	VAL
1	A	377	LEU
1	A	378	GLY
1	A	427	PRO
1	A	517	ASN
1	A	636	ASP
1	A	689	GLY
1	A	714	THR
1	A	847	LEU
1	A	975	ILE
1	A	988	PRO
1	A	991	ILE

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Mol	Chain	Res	Type
1	B	52	ALA
1	B	223	PRO
1	B	258	SER
1	B	318	PRO
1	B	357	LEU
1	B	364	ALA
1	B	597	TYR
1	B	603	LYS
1	B	654	ALA
1	B	708	LYS
1	B	765	ARG
1	B	835	LYS
1	B	936	GLY
1	B	1018	ALA
1	B	1019	ILE
1	C	33	ALA
1	C	69	MET
1	C	81	ASN
1	C	146	ASP
1	C	224	PRO
1	C	230	LEU
1	C	354	VAL
1	C	477	ALA
1	C	555	LEU
1	C	656	SER
1	C	972	LEU
1	A	236	ALA
1	A	252	LYS
1	A	287	SER
1	A	335	ILE
1	A	357	LEU
1	A	392	THR
1	A	407	ASP
1	A	416	VAL
1	A	423	GLU
1	A	439	GLN
1	A	635	ALA
1	A	693	GLU
1	A	746	ILE
1	A	892	TYR
1	A	994	GLY
1	A	1007	VAL

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Mol	Chain	Res	Type
1	B	36	PRO
1	B	82	SER
1	B	112	GLN
1	B	127	VAL
1	B	350	LEU
1	B	428	LYS
1	B	491	ALA
1	B	655	PHE
1	B	733	GLN
1	B	766	GLY
1	B	776	GLU
1	B	959	GLY
1	C	54	ALA
1	C	80	SER
1	C	206	ALA
1	C	236	ALA
1	C	372	VAL
1	C	396	PHE
1	C	410	ILE
1	C	413	VAL
1	C	425	LEU
1	C	531	VAL
1	C	617	PHE
1	C	882	ILE
1	C	895	TRP
1	C	974	PRO
1	C	982	PHE
1	A	19	ILE
1	A	50	PRO
1	A	63	GLN
1	A	120	GLN
1	A	397	GLY
1	A	832	ALA
1	A	967	ALA
1	B	171	GLY
1	B	184	MET
1	B	228	GLN
1	B	254	ASN
1	B	297	ALA
1	B	346	GLU
1	B	446	ALA
1	B	539	GLY

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Mol	Chain	Res	Type
1	B	564	LEU
1	B	713	LEU
1	B	716	VAL
1	B	723	ASP
1	B	871	ASN
1	B	957	GLY
1	B	974	PRO
1	B	992	SER
1	C	187	TRP
1	C	335	ILE
1	C	422	GLU
1	C	528	THR
1	C	636	ASP
1	C	1006	GLY
1	A	340	VAL
1	A	361	ASN
1	A	422	GLU
1	A	452	VAL
1	A	515	TRP
1	B	73	ASP
1	B	126	GLY
1	B	326	PRO
1	B	438	ILE
1	B	557	VAL
1	B	614	GLY
1	B	939	ALA
1	C	349	ILE
1	C	751	GLY
1	A	207	ILE
1	A	543	VAL
1	A	833	PRO
1	B	119	PRO
1	B	783	PRO
1	B	968	VAL
1	C	315	PRO
1	A	107	VAL
1	B	227	GLY
1	B	786	ILE
1	C	658	ILE
1	C	671	ILE
1	A	461	GLY
1	B	224	PRO

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Mol	Chain	Res	Type
1	B	621	GLY
1	A	36	PRO
1	A	140	VAL
1	C	689	GLY
1	C	935	ILE
1	A	987	MET

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%)	699 (84%)	134 (16%)	3	14
1	B	833/859 (97%)	700 (84%)	133 (16%)	3	15
1	C	833/859 (97%)	705 (85%)	128 (15%)	3	16
All	All	2499/2577 (97%)	2104 (84%)	395 (16%)	3	15

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	21	LEU
1	A	25	LEU
1	A	28	LEU
1	A	38	ILE
1	A	45	ILE
1	A	49	TYR
1	A	59	ASP
1	A	60	THR
1	A	62	THR
1	A	63	GLN
1	A	70	ASN
1	A	88	VAL
1	A	101	ASP
1	A	113	LEU
1	A	130	GLU

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Mol	Chain	Res	Type
1	A	146	ASP
1	A	161	ASN
1	A	176	GLN
1	A	181	GLN
1	A	193	LEU
1	A	207	ILE
1	A	210	GLN
1	A	214	VAL
1	A	222	THR
1	A	225	VAL
1	A	239	ARG
1	A	255	GLN
1	A	256	ASP
1	A	260	VAL
1	A	269	GLU
1	A	270	LEU
1	A	280	GLU
1	A	295	THR
1	A	298	ASN
1	A	301	ASP
1	A	310	LEU
1	A	313	MET
1	A	316	PHE
1	A	323	ILE
1	A	337	ILE
1	A	341	VAL
1	A	353	LEU
1	A	356	TYR
1	A	357	LEU
1	A	360	GLN
1	A	366	LEU
1	A	400	LEU
1	A	402	ILE
1	A	418	ARG
1	A	447	MET
1	A	448	VAL
1	A	473	THR
1	A	475	VAL
1	A	481	SER
1	A	482	VAL
1	A	489	THR
1	A	495	THR

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Mol	Chain	Res	Type
1	A	496	MET
1	A	515	TRP
1	A	526	HIS
1	A	527	TYR
1	A	530	SER
1	A	536	ARG
1	A	540	ARG
1	A	542	LEU
1	A	544	LEU
1	A	552	MET
1	A	556	PHE
1	A	562	SER
1	A	564	LEU
1	A	575	MET
1	A	576	VAL
1	A	584	GLN
1	A	612	VAL
1	A	615	PHE
1	A	620	ARG
1	A	630	SER
1	A	632	LYS
1	A	636	ASP
1	A	653	ARG
1	A	658	ILE
1	A	659	LYS
1	A	662	MET
1	A	671	ILE
1	A	674	LEU
1	A	687	GLN
1	A	702	LEU
1	A	711	ASP
1	A	712	MET
1	A	713	LEU
1	A	717	ARG
1	A	721	LEU
1	A	724	THR
1	A	739	LEU
1	A	746	ILE
1	A	750	LEU
1	A	764	ASP
1	A	773	VAL
1	A	780	ARG

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Mol	Chain	Res	Type
1	A	791	VAL
1	A	795	ASP
1	A	802	SER
1	A	806	SER
1	A	810	GLU
1	A	813	SER
1	A	843	LEU
1	A	844	MET
1	A	852	PRO
1	A	858	ASP
1	A	867	ARG
1	A	881	LEU
1	A	882	ILE
1	A	886	LEU
1	A	899	PHE
1	A	918	PHE
1	A	928	GLN
1	A	929	VAL
1	A	951	ASP
1	A	955	LYS
1	A	960	LEU
1	A	972	LEU
1	A	976	LEU
1	A	978	THR
1	A	980	LEU
1	A	982	PHE
1	A	983	ILE
1	A	986	VAL
1	A	993	THR
1	A	997	SER
1	A	1007	VAL
1	A	1021	PHE
1	A	1030	ARG
1	A	1035	ARG
1	B	11	PHE
1	B	13	TRP
1	B	21	LEU
1	B	28	LEU
1	B	49	TYR
1	B	53	ASP
1	B	57	VAL
1	B	60	THR

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Mol	Chain	Res	Type
1	B	65	ILE
1	B	67	GLN
1	B	70	ASN
1	B	74	ASN
1	B	81	ASN
1	B	83	ASP
1	B	90	ILE
1	B	91	THR
1	B	92	LEU
1	B	93	THR
1	B	95	GLU
1	B	96	SER
1	B	104	GLN
1	B	115	MET
1	B	121	GLU
1	B	128	SER
1	B	137	LEU
1	B	145	THR
1	B	148	THR
1	B	150	THR
1	B	152	GLU
1	B	154	ILE
1	B	155	SER
1	B	169	THR
1	B	176	GLN
1	B	182	TYR
1	B	185	ARG
1	B	186	ILE
1	B	189	ASN
1	B	194	ASN
1	B	199	THR
1	B	213	GLN
1	B	226	LYS
1	B	231	ASN
1	B	235	ILE
1	B	243	THR
1	B	244	GLU
1	B	250	LEU
1	B	253	VAL
1	B	254	ASN
1	B	255	GLN
1	B	259	ARG

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Mol	Chain	Res	Type
1	B	261	LEU
1	B	270	LEU
1	B	276	ASP
1	B	293	LEU
1	B	298	ASN
1	B	300	LEU
1	B	302	THR
1	B	323	ILE
1	B	329	THR
1	B	343	THR
1	B	349	ILE
1	B	356	TYR
1	B	358	PHE
1	B	372	VAL
1	B	379	THR
1	B	394	THR
1	B	395	MET
1	B	402	ILE
1	B	406	VAL
1	B	414	GLU
1	B	435	MET
1	B	456	MET
1	B	459	PHE
1	B	468	ARG
1	B	469	GLN
1	B	473	THR
1	B	478	MET
1	B	488	LEU
1	B	497	LEU
1	B	515	TRP
1	B	519	MET
1	B	528	THR
1	B	558	ARG
1	B	562	SER
1	B	564	LEU
1	B	571	VAL
1	B	587	THR
1	B	595	THR
1	B	599	LEU
1	B	601	LYS
1	B	613	ASN
1	B	620	ARG

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Mol	Chain	Res	Type
1	B	623	ASN
1	B	629	VAL
1	B	655	PHE
1	B	660	ASP
1	B	692	HIS
1	B	695	LEU
1	B	696	THR
1	B	702	LEU
1	B	714	THR
1	B	717	ARG
1	B	723	ASP
1	B	739	LEU
1	B	750	LEU
1	B	757	SER
1	B	758	TYR
1	B	773	VAL
1	B	778	LYS
1	B	779	TYR
1	B	782	LEU
1	B	795	ASP
1	B	801	PHE
1	B	808	ARG
1	B	818	ARG
1	B	826	GLU
1	B	844	MET
1	B	875	SER
1	B	880	SER
1	B	891	LEU
1	B	897	ILE
1	B	900	SER
1	B	905	VAL
1	B	914	LEU
1	B	921	LEU
1	B	935	ILE
1	B	947	GLU
1	B	952	LEU
1	B	966	ASP
1	B	972	LEU
1	B	978	THR
1	B	989	LEU
1	B	1034	SER
1	C	13	TRP

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Mol	Chain	Res	Type
1	C	30	LEU
1	C	34	GLN
1	C	35	TYR
1	C	37	THR
1	C	44	THR
1	C	46	SER
1	C	49	TYR
1	C	55	LYS
1	C	56	THR
1	C	64	VAL
1	C	68	ASN
1	C	80	SER
1	C	82	SER
1	C	84	SER
1	C	89	GLN
1	C	91	THR
1	C	96	SER
1	C	108	GLN
1	C	109	ASN
1	C	111	LEU
1	C	115	MET
1	C	118	LEU
1	C	123	GLN
1	C	128	SER
1	C	137	LEU
1	C	150	THR
1	C	151	GLN
1	C	155	SER
1	C	164	ASP
1	C	177	LEU
1	C	189	ASN
1	C	207	ILE
1	C	226	LYS
1	C	228	GLN
1	C	239	ARG
1	C	253	VAL
1	C	258	SER
1	C	259	ARG
1	C	269	GLU
1	C	274	ASN
1	C	284	GLN
1	C	285	PRO

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Mol	Chain	Res	Type
1	C	300	LEU
1	C	307	ARG
1	C	314	GLU
1	C	321	LEU
1	C	338	HIS
1	C	341	VAL
1	C	351	VAL
1	C	355	MET
1	C	370	ILE
1	C	374	VAL
1	C	377	LEU
1	C	404	LEU
1	C	417	GLU
1	C	422	GLU
1	C	425	LEU
1	C	454	VAL
1	C	459	PHE
1	C	472	ILE
1	C	480	LEU
1	C	483	LEU
1	C	497	LEU
1	C	529	ASP
1	C	542	LEU
1	C	544	LEU
1	C	555	LEU
1	C	567	GLU
1	C	571	VAL
1	C	573	MET
1	C	577	GLN
1	C	588	GLN
1	C	591	LEU
1	C	596	HIS
1	C	615	PHE
1	C	636	ASP
1	C	641	GLU
1	C	658	ILE
1	C	664	PHE
1	C	668	LEU
1	C	685	ILE
1	C	687	GLN
1	C	693	GLU
1	C	695	LEU

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Mol	Chain	Res	Type
1	C	696	THR
1	C	699	ARG
1	C	702	LEU
1	C	713	LEU
1	C	714	THR
1	C	716	VAL
1	C	722	GLU
1	C	724	THR
1	C	739	LEU
1	C	743	ILE
1	C	750	LEU
1	C	758	TYR
1	C	759	VAL
1	C	761	ASP
1	C	767	ARG
1	C	778	LYS
1	C	791	VAL
1	C	795	ASP
1	C	799	VAL
1	C	805	SER
1	C	806	SER
1	C	830	GLN
1	C	839	GLU
1	C	846	GLN
1	C	847	LEU
1	C	865	GLN
1	C	868	LEU
1	C	899	PHE
1	C	900	SER
1	C	903	LEU
1	C	914	LEU
1	C	931	LEU
1	C	935	ILE
1	C	941	ASN
1	C	952	LEU
1	C	954	ASP
1	C	960	LEU
1	C	982	PHE
1	C	983	ILE
1	C	984	LEU
1	C	993	THR
1	C	1007	VAL

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Mol	Chain	Res	Type
1	C	1036	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	58	GLN
1	A	112	GLN
1	A	120	GLN
1	A	123	GLN
1	A	124	GLN
1	A	144	ASN
1	A	210	GLN
1	A	229	GLN
1	A	231	ASN
1	A	282	ASN
1	A	298	ASN
1	A	360	GLN
1	A	577	GLN
1	A	584	GLN
1	A	622	GLN
1	A	623	ASN
1	A	709	HIS
1	A	719	ASN
1	A	726	GLN
1	A	846	GLN
1	A	865	GLN
1	A	928	GLN
1	A	1001	ASN
1	B	70	ASN
1	B	74	ASN
1	B	104	GLN
1	B	106	GLN
1	B	108	GLN
1	B	109	ASN
1	B	112	GLN
1	B	144	ASN
1	B	151	GLN
1	B	161	ASN
1	B	176	GLN
1	B	189	ASN
1	B	191	ASN

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Mol	Chain	Res	Type
1	B	210	GLN
1	B	213	GLN
1	B	218	GLN
1	B	228	GLN
1	B	231	ASN
1	B	254	ASN
1	B	391	ASN
1	B	415	ASN
1	B	517	ASN
1	B	613	ASN
1	B	622	GLN
1	B	700	ASN
1	B	709	HIS
1	B	726	GLN
1	B	733	GLN
1	B	846	GLN
1	B	872	GLN
1	B	941	ASN
1	C	3	ASN
1	C	34	GLN
1	C	58	GLN
1	C	63	GLN
1	C	89	GLN
1	C	144	ASN
1	C	176	GLN
1	C	189	ASN
1	C	197	GLN
1	C	211	ASN
1	C	213	GLN
1	C	231	ASN
1	C	237	GLN
1	C	274	ASN
1	C	284	GLN
1	C	360	GLN
1	C	439	GLN
1	C	577	GLN
1	C	588	GLN
1	C	605	ASN
1	C	700	ASN
1	C	737	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 carbohydrates 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	ERY	C	3402	-	53,53,53	0.98	1 (1%)	82,82,82	1.67	19 (23%)

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	ERY	C	3402	-	-	0/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3402	ERY	O2-C1	4.89	1.45	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3402	ERY	C13-O2-C1	-3.38	112.42	118.12
2	C	3402	ERY	O12-C11-C12	-3.03	101.69	106.79
2	C	3402	ERY	C25-C24-N1	-3.02	106.77	115.70
2	C	3402	ERY	C33-C8-C7	-2.69	104.06	109.69
2	C	3402	ERY	O7-C5-C4	-2.34	107.65	111.48
2	C	3402	ERY	C34-C10-C11	-2.25	111.55	114.46
2	C	3402	ERY	O2-C1-O1	-2.23	119.31	123.89
2	C	3402	ERY	O7-C22-O9	-2.15	105.23	110.68
2	C	3402	ERY	C6-C5-C4	-2.04	111.24	114.11
2	C	3402	ERY	C29-N1-C28	2.02	116.81	110.43
2	C	3402	ERY	C25-C24-C23	2.10	113.08	110.03
2	C	3402	ERY	O7-C22-C23	2.16	113.35	108.10
2	C	3402	ERY	O4-C18-C21	2.52	112.15	106.64
2	C	3402	ERY	O7-C5-C6	3.02	110.29	106.44
2	C	3402	ERY	O12-C11-C10	3.11	115.38	110.78
2	C	3402	ERY	C20-O5-C16	3.70	126.23	117.72
2	C	3402	ERY	O2-C1-C2	3.81	119.29	111.47
2	C	3402	ERY	C29-N1-C24	3.90	124.37	113.09
2	C	3402	ERY	C15-C16-C17	4.76	113.78	107.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3402	ERY	10	0

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	39 (3%)	44	43	58, 111, 150, 192	0
1	B	1022/1053 (97%)	0.24	51 (4%)	32	32	69, 115, 154, 179	0
1	C	1022/1053 (97%)	0.19	46 (4%)	37	36	55, 109, 160, 188	0
All	All	3066/3159 (97%)	0.21	136 (4%)	38	37	55, 113, 155, 192	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	520	PHE	9.7
1	A	497	LEU	5.8
1	B	963	ALA	5.6
1	C	537	SER	5.3
1	A	259	ARG	4.7
1	C	540	ARG	4.7
1	C	712	MET	4.3
1	C	1034	SER	4.2
1	A	515	TRP	4.2
1	B	675	GLY	4.2
1	B	1033	PHE	3.9
1	A	1036	LYS	3.9
1	C	538	THR	3.9
1	C	425	LEU	3.9
1	B	515	TRP	3.8
1	B	676	THR	3.8
1	A	513	PHE	3.8
1	C	872	GLN	3.8
1	C	671	ILE	3.7
1	C	535	LEU	3.6
1	C	497	LEU	3.6
1	A	198	LEU	3.6
1	C	962	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	539	GLY	3.5
1	B	420	MET	3.5
1	C	1033	PHE	3.5
1	B	526	HIS	3.4
1	B	635	ALA	3.4
1	B	727	PHE	3.3
1	B	435	MET	3.2
1	A	425	LEU	3.2
1	A	419	VAL	3.2
1	A	253	VAL	3.1
1	C	420	MET	3.1
1	C	604	ASN	3.1
1	B	426	PRO	3.1
1	B	779	TYR	3.0
1	C	496	MET	3.0
1	A	145	THR	3.0
1	C	515	TRP	2.9
1	A	1029	VAL	2.9
1	C	516	PHE	2.9
1	B	497	LEU	2.9
1	A	258	SER	2.9
1	B	188	MET	2.9
1	C	675	GLY	2.8
1	C	252	LYS	2.8
1	C	430	ALA	2.8
1	C	961	ILE	2.8
1	A	427	PRO	2.8
1	B	634	TRP	2.7
1	B	964	THR	2.7
1	B	949	ALA	2.7
1	B	670	ALA	2.7
1	A	1030	ARG	2.7
1	A	1033	PHE	2.7
1	A	149	MET	2.7
1	B	669	PRO	2.7
1	B	597	TYR	2.6
1	B	494	ALA	2.6
1	A	322	LYS	2.6
1	A	712	MET	2.6
1	C	251	LEU	2.6
1	A	431	THR	2.6
1	A	230	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	514	GLY	2.6
1	B	516	PHE	2.6
1	C	957	GLY	2.5
1	B	679	GLY	2.5
1	C	606	VAL	2.5
1	A	199	THR	2.5
1	A	154	ILE	2.5
1	A	31	PRO	2.5
1	A	134	SER	2.5
1	C	424	GLY	2.5
1	C	431	THR	2.5
1	A	558	ARG	2.5
1	B	363	ARG	2.5
1	B	535	LEU	2.5
1	C	423	GLU	2.4
1	B	804	PHE	2.4
1	C	900	SER	2.4
1	C	357	LEU	2.4
1	C	427	PRO	2.4
1	C	459	PHE	2.4
1	B	493	CYS	2.4
1	A	698	ALA	2.4
1	A	142	VAL	2.4
1	B	672	VAL	2.4
1	C	641	GLU	2.3
1	B	3	ASN	2.3
1	B	606	VAL	2.3
1	B	554	TYR	2.3
1	C	361	ASN	2.3
1	A	287	SER	2.3
1	A	964	THR	2.3
1	C	871	ASN	2.3
1	C	895	TRP	2.3
1	B	847	LEU	2.3
1	B	918	PHE	2.3
1	B	660	ASP	2.3
1	A	196	PHE	2.3
1	B	412	VAL	2.3
1	A	32	VAL	2.2
1	B	991	ILE	2.2
1	B	134	SER	2.2
1	C	259	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	188	MET	2.2
1	A	265	VAL	2.2
1	C	264	ASP	2.2
1	C	676	THR	2.2
1	B	647	ILE	2.2
1	A	958	LYS	2.2
1	C	897	ILE	2.2
1	B	993	THR	2.2
1	B	604	ASN	2.2
1	B	1	MET	2.2
1	A	321	LEU	2.2
1	A	426	PRO	2.2
1	B	133	SER	2.1
1	B	321	LEU	2.1
1	A	1031	ARG	2.1
1	C	498	LYS	2.1
1	C	741	VAL	2.1
1	B	843	LEU	2.1
1	B	1005	THR	2.1
1	C	536	ARG	2.1
1	B	148	THR	2.1
1	B	553	ALA	2.1
1	B	417	GLU	2.1
1	B	682	PHE	2.1
1	B	1034	SER	2.1
1	B	678	THR	2.1
1	A	713	LEU	2.1
1	A	967	ALA	2.0
1	C	262	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ERY	C	3402	51/51	0.85	0.33	1.19	58,68,74,79	51

6.5 Other polymers [i](#)

There are no such residues in this entry.