



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:28 AM UTC

PDB ID : 3AOD / pdb_00003aod
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 : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

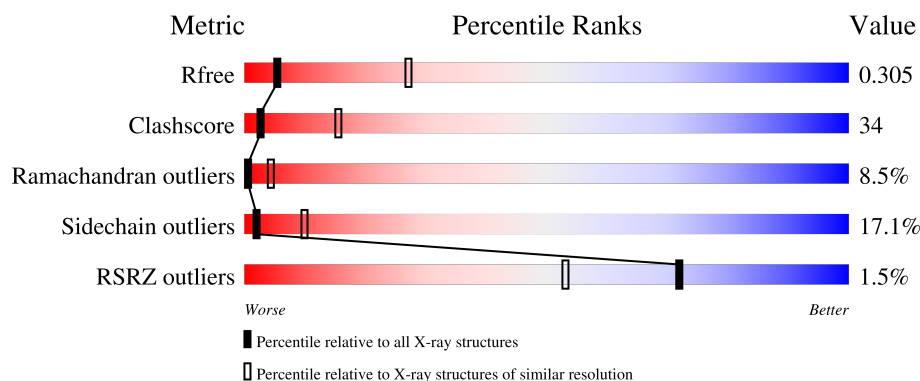
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1053	% 40% 43% 12% ..
1	B	1053	2% 39% 44% 13% ..
1	C	1053	% 41% 43% 12% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23419 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.

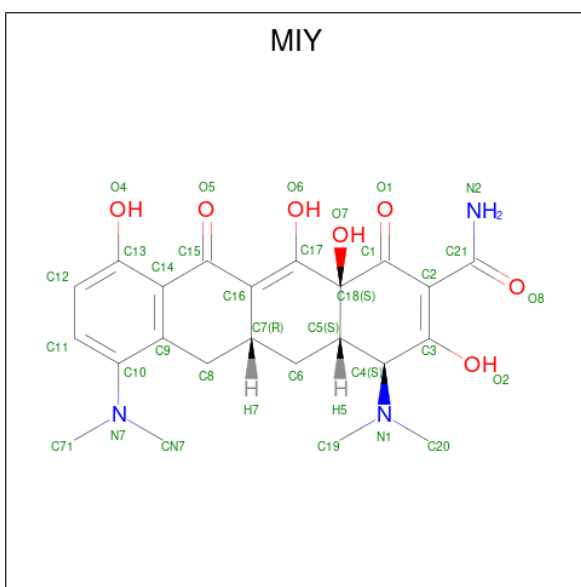
- Molecule 1 is a protein called Acriflavine resistance protein B.

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:

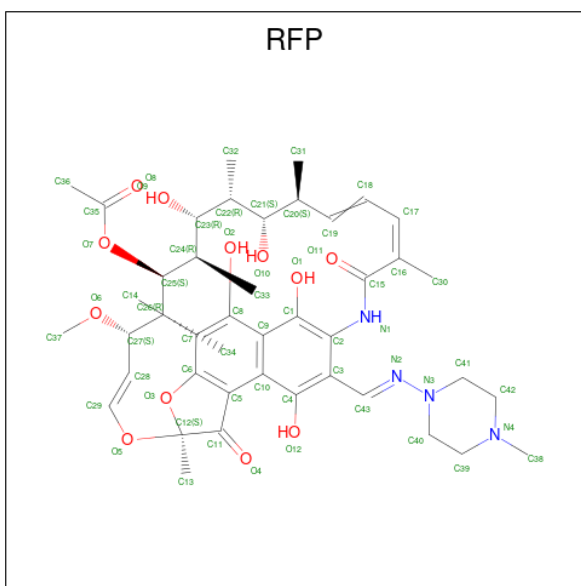
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
B	1051	HIS	-	expression tag	UNP P31224
B	1052	HIS	-	expression 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 (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: MIY) (formula: $C_{23}H_{27}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	23	3	7		

- Molecule 3 is RIFAMPICIN (CCD ID: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



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

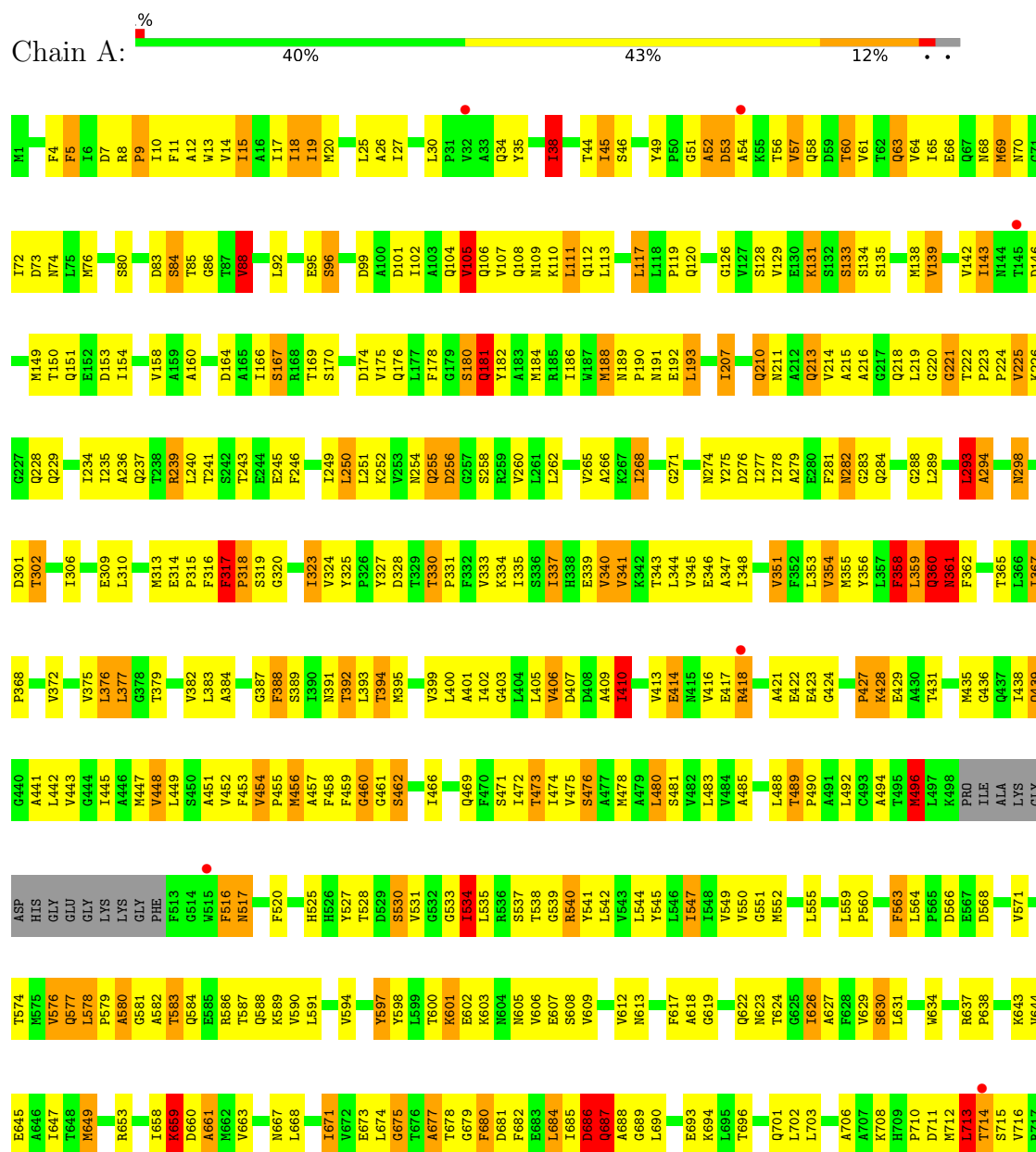
- Molecule 4 is water.

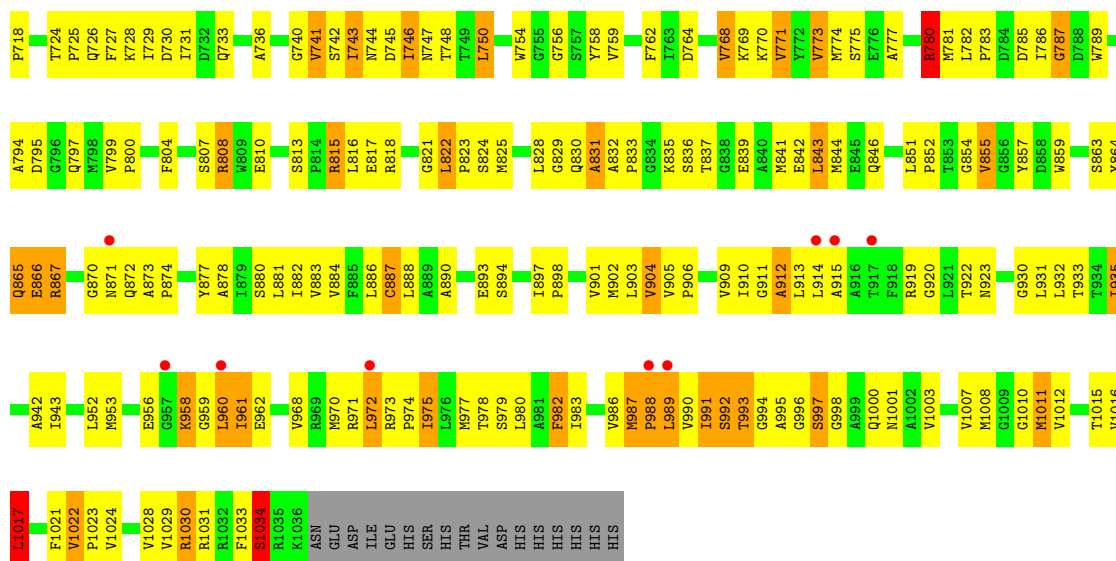
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	2	Total 2	O 2	0	0
4	C	1	Total 1	O 1	0	0

3 Residue-property plots

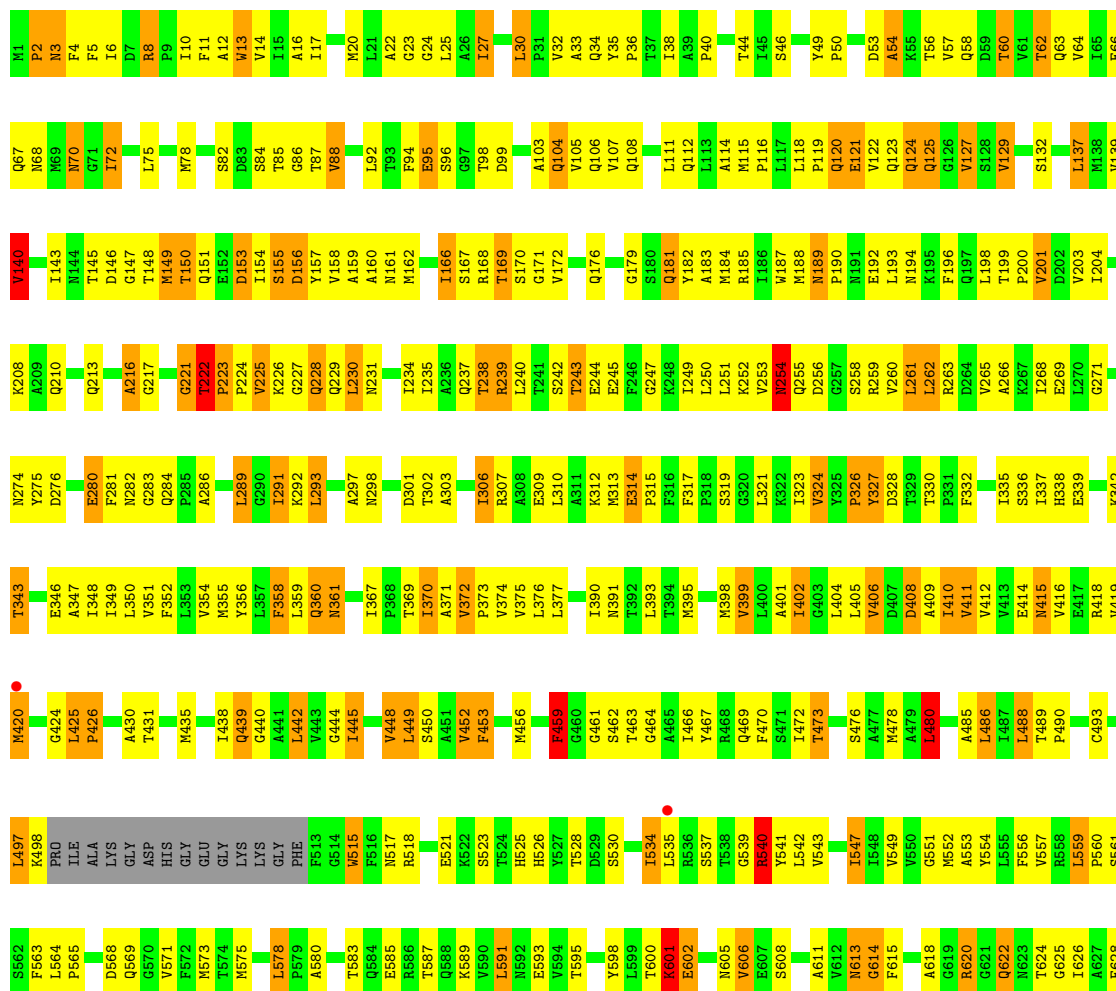
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

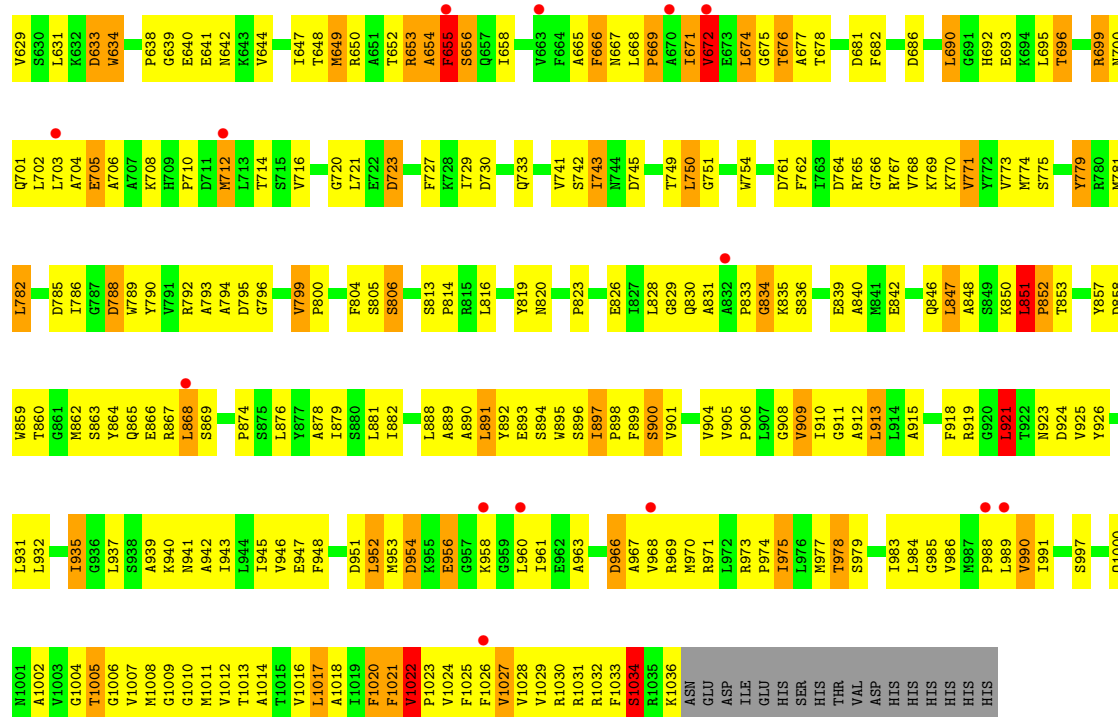
• Molecule 1: Acriflavine resistance protein B



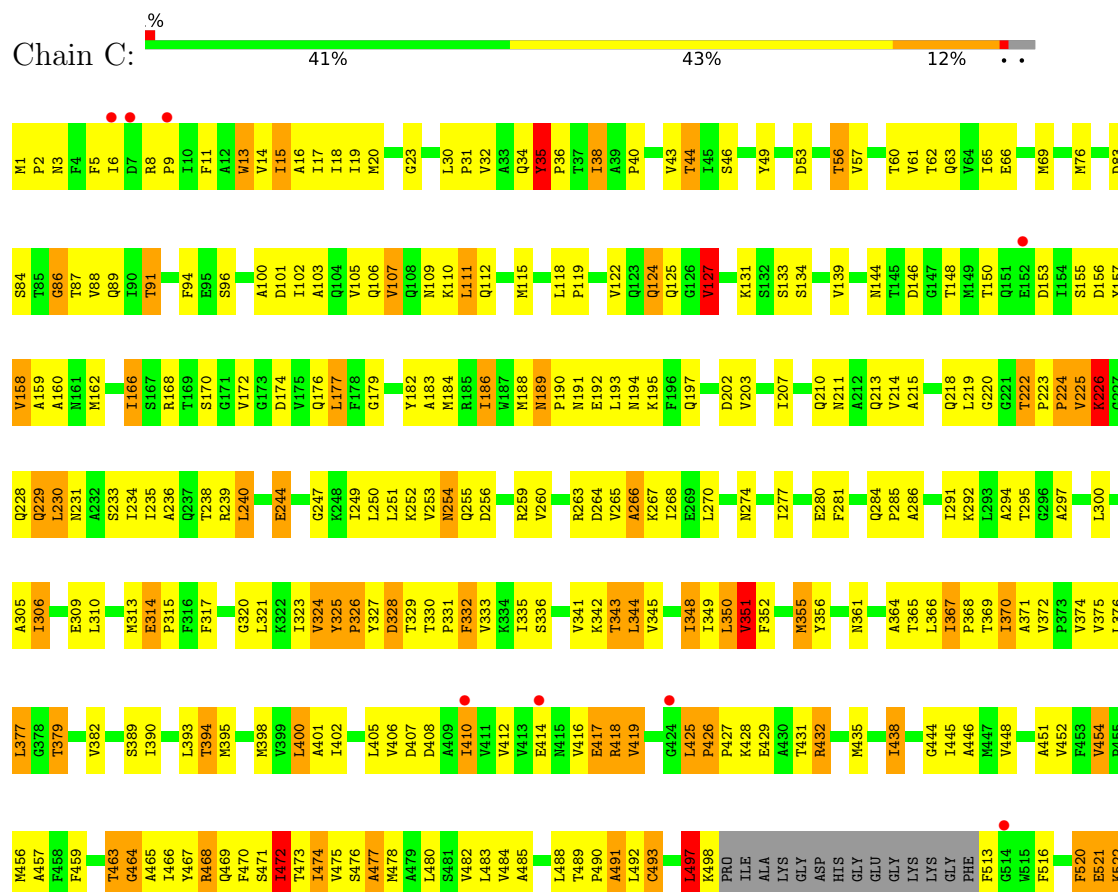


• Molecule 1: Acriflavine resistance protein B





- Molecule 1: Acriflavine resistance protein B



ILE	R973	L907	G834	V759	L690	V606	S523
	GLU	G908	K835	N760	G691	E607	T524
	HIS	V909	S836	D761	H692	E607	H525
	SER	L976	L976	F762	E693	S608	H526
	HIS	K977	G911	L763	K694	V609	Y527
	THR			D764	L695	F610	T528
	VAL	F982	L914	R765	T696	A611	D529
	ASP	L983	A915	G766	R767	S630	S530
	HIS	L984	L843	R768	A698		V631
	HIS	L985	R919	V768	R699	R620	
HIS	Y986	G920	K847	K769	M623	M623	L534
	K987	L921	S849	D770	T624	T624	L535
	P988	T922	K850	V771			
	Y990	V925	L851	M774	A707	F628	T538
		Y926		S775	P710	V629	G539
	T993	F927	G854	E776	D711	L631	Y541
	G994	Q928	V855	A777	M712	K632	L542
		V929	G856	K778	L713	D633	V543
	S997	G930	V857	Y779	T714	M634	L544
	G998	L931	R857	R780	S715	A635	
HIS	A999	L932	D858	M781	V716	D636	M552
	Q1000	T933	M859	L782	R717	R637	A553
		R934		P783			Y554
	G1004	L935	S863	D784	G720	M642	L555
	T1005	G936	Y864	L785	L721	K643	F556
	G1006		Q865	D786	E722	V644	V557
	V1007	K940	E866	M789	T723	L647	R558
	M1008	N941	R867	D790	D724	T648	F563
	G1009	A942	L868	V790		M649	L564
	M1010	L943	S869	V991	F727		
HIS	G1011	L944	G870	R792	K728		D568
	V1012	L945	N871	D795	T729	F655	Q569
	T1013	V946	Q872	D795	D730	S656	G570
	A1014	F947	A873	G796	I731	O657	V571
	T1015	F948	P874	Q797	D732	L658	
	V1016	A949	S875	N798	Q733		T574
	L1017	K950	L876	V799	E734	F664	M575
	A1018	D951	I879	P800	K735	M682	V576
	L1019	L952	R952	F801	A736	V663	Q577
	F1020	M953	G802	L803	Q737	F664	L578
HIS	F1021	D954	V883	S803	A738	A685	P579
	V1022	K955	V894	F804	L739		A580
	P1023	E956	F885	S805	G740		T583
	V1024	G957	S806	S806	V741	V672	
	F1025	K958	L888	S907	E673	E673	Q588
	G959	A889	A889	R808	I743	L674	K589
	V1026	F960	A890		R744	G675	L591
	V1027	L960		P814	D745		
	V1028	L961	E893	R815	I746	T678	
	V1029	E962		A963	L750	G679	Q590
HIS	R1030	A963	S896	G821	F751	F690	H596
	L1031	T964	L965	L822	A752	D681	Y597
	R1032	L965					Y598
	F1033	D966	F899	M825	A753	L684	L599
	A1034	A967	S900		W754	T685	T600
	R1035	V968	V901			D686	K601
	K1036	R969	Q830	Q830	G756	Q637	
	ASN	M970	V904	A831	G756	A658	E602
	GLU	R971	A832	R832	V757	C650	K602
	ASP	L972	D905	D923			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.60Å 134.50Å 162.83Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	47.50 – 3.30 47.50 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.50-3.30) 97.2 (47.50-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.67 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.258 , 0.318 0.251 , 0.305	Depositor DCC
R_{free} test set	3532 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	95.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23419	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.84	2/7920 (0.0%)	1.10	30/10756 (0.3%)
1	B	0.79	2/7920 (0.0%)	1.09	17/10756 (0.2%)
1	C	0.85	1/7920 (0.0%)	1.13	33/10756 (0.3%)
All	All	0.82	5/23760 (0.0%)	1.11	80/32268 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1022	VAL	CA-CB	7.89	1.59	1.53
1	B	897	ILE	CA-CB	6.55	1.58	1.53
1	C	671	ILE	CA-CB	6.16	1.62	1.54
1	B	672	VAL	CA-CB	5.06	1.61	1.54
1	A	768	VAL	CA-CB	-5.03	1.48	1.54

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	351	VAL	N-CA-C	-10.29	103.93	113.71
1	B	459	PHE	N-CA-C	9.36	120.26	108.19
1	B	425	LEU	CA-C-N	9.12	129.78	120.38
1	B	425	LEU	C-N-CA	9.12	129.78	120.38
1	C	864	TYR	N-CA-C	-8.12	103.31	113.55
1	C	426	PRO	N-CA-C	8.09	120.56	110.70
1	A	361	ASN	N-CA-C	7.54	117.16	108.49
1	B	221	GLY	N-CA-C	7.46	120.53	112.33
1	B	352	PHE	N-CA-C	-7.30	104.50	113.41
1	C	309	GLU	N-CA-C	-7.17	102.66	111.40
1	C	254	ASN	N-CA-C	7.12	119.12	107.23
1	C	284	GLN	CA-C-N	6.89	128.45	119.84
1	C	284	GLN	C-N-CA	6.89	128.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	VAL	N-CA-C	-6.69	102.76	110.05
1	B	426	PRO	N-CA-C	6.66	118.83	110.70
1	B	921	LEU	N-CA-C	6.63	119.63	110.35
1	C	776	GLU	N-CA-C	-6.55	101.70	110.55
1	C	491	ALA	N-CA-C	-6.50	102.14	110.19
1	C	166	ILE	N-CA-C	-6.46	104.19	110.72
1	C	925	VAL	N-CA-C	-6.45	104.46	110.53
1	C	659	LYS	N-CA-C	6.41	116.53	108.45
1	B	222	THR	CA-C-N	6.38	126.95	120.38
1	B	222	THR	C-N-CA	6.38	126.95	120.38
1	A	96	SER	N-CA-C	6.27	121.15	111.56
1	C	746	ILE	CB-CA-C	-6.26	103.99	111.81
1	B	771	VAL	CB-CA-C	-6.14	103.42	110.73
1	A	807	SER	N-CA-C	6.13	118.40	108.41
1	A	239	ARG	N-CA-C	6.06	118.78	110.24
1	A	222	THR	N-CA-C	-6.01	101.49	109.84
1	B	254	ASN	N-CA-C	5.98	119.20	110.17
1	C	1034	SER	N-CA-C	-5.88	104.98	113.21
1	C	35	TYR	N-CA-C	-5.84	99.43	108.55
1	A	644	VAL	N-CA-C	5.83	116.48	110.82
1	C	759	VAL	N-CA-C	5.83	116.05	110.74
1	C	428	LYS	N-CA-C	5.75	117.22	111.07
1	A	88	VAL	CB-CA-C	-5.73	102.08	110.62
1	B	897	ILE	N-CA-CB	5.72	114.10	110.50
1	C	685	ILE	N-CA-C	5.71	116.97	108.46
1	A	771	VAL	CB-CA-C	-5.71	104.75	111.09
1	A	146	ASP	N-CA-C	-5.67	108.16	114.62
1	A	912	ALA	N-CA-C	-5.67	105.01	111.07
1	A	188	MET	N-CA-C	5.66	118.05	110.35
1	C	229	GLN	N-CA-C	-5.64	102.12	110.46
1	C	49	TYR	CA-C-N	5.63	126.88	119.84
1	C	49	TYR	C-N-CA	5.63	126.88	119.84
1	C	830	GLN	N-CA-C	5.61	116.48	108.74
1	A	687	GLN	N-CA-C	5.59	122.70	110.80
1	A	686	ASP	N-CA-C	5.58	120.58	113.55
1	A	218	GLN	CA-C-O	5.56	121.16	117.94
1	B	634	TRP	N-CA-C	5.56	118.18	111.40
1	A	871	ASN	N-CA-C	-5.54	106.57	113.55
1	C	474	ILE	N-CA-C	5.52	116.25	110.62
1	A	45	ILE	CB-CA-C	-5.47	103.40	110.84
1	B	1022	VAL	N-CA-CB	5.46	114.71	110.45
1	C	720	GLY	N-CA-C	5.45	126.11	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ALA	N-CA-C	5.45	117.92	111.33
1	C	214	VAL	N-CA-C	5.44	115.82	107.77
1	C	986	VAL	N-CA-C	-5.41	105.65	113.07
1	A	997	SER	O-C-N	5.37	124.80	120.83
1	C	277	ILE	N-CA-C	5.32	115.18	106.72
1	A	222	THR	CB-CA-C	5.31	118.17	109.46
1	A	317	PHE	CA-C-N	5.31	126.47	119.84
1	A	317	PHE	C-N-CA	5.31	126.47	119.84
1	A	864	TYR	N-CA-C	-5.27	105.92	112.93
1	C	270	LEU	N-CA-C	-5.26	101.40	109.76
1	A	780	ARG	N-CA-C	5.25	116.74	110.44
1	A	581	GLY	N-CA-C	5.24	120.44	114.67
1	B	23	GLY	N-CA-C	-5.21	105.94	111.93
1	C	493	CYS	N-CA-C	-5.20	104.63	111.96
1	A	915	ALA	N-CA-C	-5.18	106.81	112.72
1	A	1022	VAL	N-CA-CB	5.11	113.72	110.50
1	B	480	LEU	N-CA-C	-5.09	106.76	113.12
1	A	855	VAL	N-CA-C	5.08	116.11	109.21
1	A	105	VAL	CB-CA-C	-5.07	102.98	111.29
1	A	777	ALA	CA-C-N	5.04	127.29	120.38
1	A	777	ALA	C-N-CA	5.04	127.29	120.38
1	C	472	ILE	N-CA-C	5.04	115.66	110.36
1	C	374	VAL	N-CA-C	-5.01	105.96	110.82
1	B	166	ILE	N-CA-C	-5.00	105.83	110.53
1	C	314	GLU	O-C-N	5.00	124.33	120.38

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	548	0
1	B	7774	0	7931	577	0
1	C	7774	0	7931	542	0
2	A	33	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	59	0	56	5	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
All	All	23419	0	23873	1599	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (1599) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LEU:CB	1:A:832:ALA:HA	1.80	1.11
1:C:44:THR:HG23	1:C:91:THR:HB	1.33	1.10
1:C:909:VAL:HG12	1:C:931:LEU:HD21	1.11	1.09
1:B:95:GLU:O	1:B:98:THR:HG22	1.50	1.09
1:C:115:MET:HE2	1:C:118:LEU:HD23	1.38	1.05
1:A:713:LEU:HB3	1:A:832:ALA:HA	1.09	1.03
1:B:1026:PHE:HB3	1:B:1030:ARG:HH21	1.23	1.02
1:A:901:VAL:O	1:A:904:VAL:HG23	1.60	1.02
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.42	1.01
1:C:713:LEU:HD11	1:C:834:GLY:HA3	1.02	1.01
1:B:222:THR:HB	1:B:223:PRO:HD3	1.38	1.01
1:B:573:MET:HE3	1:B:575:MET:HE1	1.41	1.01
1:A:713:LEU:HB3	1:A:832:ALA:CA	1.89	1.01
1:C:760:ASN:O	1:C:771:VAL:HG23	1.61	1.01
1:B:919:ARG:HD2	1:B:1005:THR:HG21	1.42	1.00
1:A:671:ILE:H	1:A:671:ILE:CD1	1.74	1.00
1:C:184:MET:HA	1:C:184:MET:HE3	1.39	1.00
1:C:713:LEU:CD1	1:C:834:GLY:HA3	1.92	0.98
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.44	0.98
1:C:190:PRO:HD2	1:C:779:TYR:CD1	1.99	0.97
1:A:30:LEU:HD21	1:A:384:ALA:HB2	1.46	0.96
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.47	0.96
1:C:950:LYS:HA	1:C:953:MET:HE2	1.47	0.96
1:A:731:ILE:HG12	1:A:746:ILE:HG21	1.49	0.94
1:C:418:ARG:HH22	1:C:970:MET:HE2	1.30	0.94
1:A:659:LYS:HD2	1:A:660:ASP:H	1.33	0.93
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.50	0.93
1:A:356:TYR:HD1	1:A:361:ASN:H	1.17	0.93
1:A:713:LEU:HG	1:A:833:PRO:HD3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:GLY:H	1:A:914:LEU:HD13	1.34	0.92
1:C:162:MET:HA	1:C:313:MET:HE1	1.50	0.92
1:B:835:LYS:HB2	1:B:839:GLU:OE2	1.70	0.91
1:A:73:ASP:H	1:A:106:GLN:HE22	1.10	0.91
1:C:1025:PHE:O	1:C:1029:VAL:HB	1.70	0.91
1:C:115:MET:CE	1:C:127:VAL:HG11	2.00	0.91
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.52	0.90
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.50	0.89
1:C:758:TYR:HE2	1:C:770:LYS:HB3	1.34	0.89
1:C:564:LEU:HD13	1:C:671:ILE:HD12	1.54	0.89
1:A:713:LEU:HB2	1:A:833:PRO:HD3	1.54	0.89
1:C:211:ASN:HD22	1:C:240:LEU:HG	1.38	0.89
1:A:395:MET:HE2	1:A:395:MET:HA	1.54	0.88
1:C:758:TYR:CE2	1:C:770:LYS:HB3	2.08	0.88
1:A:302:THR:O	1:A:306:ILE:HG12	1.73	0.88
1:A:462:SER:HB2	1:A:865:GLN:HG2	1.56	0.88
1:B:222:THR:HB	1:B:223:PRO:CD	2.03	0.88
1:C:848:ALA:HA	1:C:851:LEU:HD22	1.56	0.88
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.56	0.88
1:B:463:THR:HG21	1:B:869:SER:HB2	1.54	0.88
1:B:729:ILE:HG13	1:B:730:ASP:H	1.37	0.88
1:A:886:LEU:HD21	1:C:17:ILE:HG22	1.54	0.87
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.56	0.87
1:B:897:ILE:HB	1:B:1026:PHE:HE1	1.40	0.87
1:C:1:MET:HB2	1:C:2:PRO:CD	2.04	0.86
1:C:418:ARG:HH12	1:C:970:MET:HG2	1.39	0.86
1:C:758:TYR:CE2	1:C:770:LYS:HD3	2.09	0.86
1:A:447:MET:HB3	1:A:887:CYS:SG	2.16	0.86
1:A:14:VAL:HG21	1:B:890:ALA:HB2	1.55	0.86
1:A:15:ILE:O	1:A:19:ILE:HD13	1.73	0.86
1:C:281:PHE:CZ	1:C:324:VAL:HG21	2.11	0.86
1:B:150:THR:H	1:B:153:ASP:HB2	1.41	0.85
1:A:310:LEU:HD12	1:A:325:TYR:OH	1.76	0.85
1:C:848:ALA:HA	1:C:851:LEU:CD2	2.07	0.85
1:A:886:LEU:HG	1:C:14:VAL:HG23	1.57	0.85
1:A:886:LEU:HD21	1:C:17:ILE:CG2	2.06	0.84
1:A:454:VAL:HG12	1:A:455:PRO:HD3	1.57	0.84
1:B:560:PRO:HB2	1:B:836:SER:HB3	1.60	0.84
1:C:485:ALA:O	1:C:490:PRO:HD3	1.77	0.84
1:B:459:PHE:HZ	1:B:876:LEU:HG	1.40	0.83
1:B:416:VAL:HG11	1:B:431:THR:HG22	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:LEU:HD11	1:C:834:GLY:CA	1.98	0.83
1:B:70:ASN:H	1:B:70:ASN:HD22	1.27	0.83
1:B:84:SER:HB3	1:B:814:PRO:HA	1.59	0.83
1:A:11:PHE:CD1	1:B:890:ALA:HB1	2.13	0.83
1:B:1020:PHE:O	1:B:1021:PHE:HB2	1.76	0.83
1:C:729:ILE:HD11	1:C:786:ILE:CD1	2.09	0.82
1:B:104:GLN:HE21	1:B:104:GLN:C	1.87	0.82
1:C:418:ARG:NH2	1:C:970:MET:HE2	1.92	0.82
1:C:901:VAL:O	1:C:904:VAL:HG23	1.81	0.80
1:A:852:PRO:O	1:A:855:VAL:HG22	1.81	0.80
1:C:38:ILE:HD13	1:C:38:ILE:H	1.45	0.80
1:C:775:SER:HB3	1:C:780:ARG:HD3	1.63	0.80
1:B:743:ILE:HD13	1:B:743:ILE:H	1.44	0.80
1:B:906:PRO:HA	1:B:909:VAL:HG22	1.63	0.80
1:C:729:ILE:HD11	1:C:786:ILE:HD13	1.63	0.79
1:C:34:GLN:HB3	1:C:333:VAL:CG2	2.12	0.79
1:C:189:ASN:C	1:C:189:ASN:HD22	1.90	0.79
1:A:367:ILE:HG22	1:A:496:MET:HE1	1.64	0.79
1:A:843:LEU:HA	1:A:846:GLN:HE21	1.47	0.79
1:C:696:THR:O	1:C:699:ARG:HG3	1.82	0.79
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.64	0.79
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.13	0.79
1:C:418:ARG:HH22	1:C:970:MET:CE	1.96	0.78
1:C:909:VAL:HG12	1:C:931:LEU:CD2	2.05	0.78
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.65	0.78
1:A:4:PHE:O	1:A:8:ARG:NH2	2.16	0.78
1:A:713:LEU:CB	1:A:833:PRO:HD3	2.14	0.78
1:A:690:LEU:HD11	1:A:854:GLY:HA3	1.65	0.78
1:C:115:MET:HE1	1:C:127:VAL:HG11	1.65	0.78
1:A:671:ILE:H	1:A:671:ILE:HD13	1.47	0.78
1:A:756:GLY:HA2	1:A:774:MET:HB3	1.65	0.78
1:A:1011:MET:HE3	1:A:1011:MET:HA	1.66	0.78
1:A:886:LEU:O	1:C:14:VAL:HG21	1.84	0.77
1:A:601:LYS:O	1:A:601:LYS:HG3	1.83	0.77
1:A:104:GLN:HE21	1:A:131:LYS:HD3	1.50	0.77
1:A:878:ALA:O	1:A:882:ILE:HD13	1.85	0.77
1:A:987:MET:H	1:A:988:PRO:HD3	1.47	0.77
1:A:126:GLY:HA3	1:B:116:PRO:HB3	1.66	0.77
1:A:832:ALA:CB	1:A:835:LYS:HB2	2.14	0.77
1:B:94:PHE:HB3	1:B:98:THR:HG21	1.65	0.77
1:B:743:ILE:HD13	1:B:743:ILE:N	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:MET:HE2	1:C:118:LEU:CD2	2.13	0.77
1:A:383:LEU:HD21	1:A:473:THR:HG23	1.66	0.77
1:B:139:VAL:HG12	1:B:139:VAL:O	1.83	0.77
1:A:680:PHE:CZ	1:A:844:MET:HE2	2.20	0.76
1:B:591:LEU:O	1:B:595:THR:HG22	1.85	0.76
1:C:343:THR:HG21	1:C:989:LEU:HD13	1.65	0.76
1:C:974:PRO:HA	1:C:977:MET:HE3	1.67	0.76
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.15	0.76
1:B:54:ALA:HB1	1:B:816:LEU:HD12	1.67	0.76
1:B:1020:PHE:N	1:B:1020:PHE:HD2	1.84	0.76
1:A:219:LEU:HD22	1:B:781:MET:O	1.86	0.76
1:A:987:MET:N	1:A:988:PRO:HD3	2.01	0.76
1:B:867:ARG:HG2	1:B:868:LEU:HD22	1.68	0.76
1:B:1026:PHE:HB3	1:B:1030:ARG:NH2	2.01	0.76
1:A:713:LEU:HD22	1:A:714:THR:H	1.51	0.75
1:A:466:ILE:O	1:A:469:GLN:HB2	1.86	0.75
1:A:729:ILE:HG22	1:A:730:ASP:N	2.01	0.75
1:A:775:SER:O	1:A:780:ARG:HD3	1.86	0.75
1:A:538:THR:H	1:A:540:ARG:NH2	1.84	0.75
1:A:457:ALA:O	1:A:458:PHE:HD1	1.68	0.75
1:C:444:GLY:O	1:C:448:VAL:HG23	1.87	0.75
1:A:13:TRP:O	1:A:17:ILE:HG12	1.86	0.75
1:A:367:ILE:HD11	1:A:413:VAL:HB	1.68	0.74
1:C:184:MET:HA	1:C:184:MET:CE	2.17	0.74
1:A:533:GLY:C	1:A:535:LEU:H	1.95	0.74
1:A:987:MET:O	1:A:987:MET:HG2	1.86	0.74
1:B:699:ARG:O	1:B:701:GLN:N	2.20	0.74
1:A:268:ILE:O	1:A:268:ILE:HG22	1.86	0.74
1:B:6:ILE:HD11	1:B:490:PRO:HB2	1.68	0.74
1:C:643:LYS:O	1:C:647:ILE:HG13	1.87	0.74
1:B:573:MET:CE	1:B:575:MET:HE1	2.16	0.74
1:C:395:MET:HE2	1:C:395:MET:HA	1.69	0.74
1:C:909:VAL:CG1	1:C:931:LEU:HD21	2.06	0.74
1:B:898:PRO:C	1:B:900:SER:H	1.96	0.73
1:A:11:PHE:HD1	1:B:890:ALA:HB1	1.51	0.73
1:A:52:ALA:HB3	1:A:86:GLY:HA2	1.71	0.73
1:B:171:GLY:HA3	1:B:302:THR:CB	2.19	0.73
1:B:652:THR:O	1:B:656:SER:HB3	1.88	0.73
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.70	0.73
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.54	0.73
1:C:379:THR:HB	1:C:398:MET:HE2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LYS:HG2	1:C:260:VAL:CG1	2.18	0.73
1:A:52:ALA:HB1	1:A:57:VAL:HG23	1.71	0.72
1:B:280:GLU:HB2	1:B:284:GLN:O	1.88	0.72
1:B:699:ARG:HH11	1:B:699:ARG:HB3	1.54	0.72
1:C:758:TYR:HE2	1:C:770:LYS:HD3	1.54	0.72
1:B:171:GLY:HA3	1:B:302:THR:HB	1.71	0.72
1:B:1020:PHE:N	1:B:1020:PHE:CD2	2.55	0.72
1:C:554:TYR:O	1:C:556:PHE:N	2.22	0.72
1:B:671:ILE:HG22	1:B:672:VAL:N	2.03	0.72
1:A:584:GLN:HB2	1:A:622:GLN:HG2	1.70	0.72
1:A:808:ARG:H	1:A:808:ARG:HD2	1.53	0.72
1:A:80:SER:OG	1:A:818:ARG:HG3	1.90	0.72
1:A:795:ASP:OD1	1:A:797:GLN:HG2	1.88	0.72
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.71	0.71
1:A:990:VAL:O	1:A:991:ILE:HG12	1.90	0.71
1:A:5:PHE:CE1	1:A:12:ALA:HB2	2.25	0.71
1:A:216:ALA:HB2	1:B:750:LEU:HD13	1.72	0.71
1:B:986:VAL:O	1:B:990:VAL:HG23	1.90	0.71
1:B:158:VAL:HA	1:B:162:MET:CG	2.20	0.71
1:B:701:GLN:HB3	1:B:851:LEU:HD13	1.73	0.71
1:A:142:VAL:O	1:A:154:ILE:HG21	1.90	0.71
1:A:671:ILE:H	1:A:671:ILE:HD12	1.53	0.71
1:B:188:MET:HE1	1:B:200:PRO:HA	1.72	0.71
1:A:733:GLN:OE1	1:A:743:ILE:HD11	1.91	0.71
1:B:979:SER:O	1:B:983:ILE:HG13	1.90	0.71
1:A:53:ASP:HA	1:A:84:SER:HA	1.73	0.71
1:A:73:ASP:H	1:A:106:GLN:NE2	1.87	0.71
1:C:524:THR:HG22	1:C:972:LEU:HD12	1.73	0.71
1:A:178:PHE:HB2	1:A:288:GLY:H	1.55	0.70
1:C:911:GLY:HA3	1:C:1013:THR:HG21	1.73	0.70
1:A:1029:VAL:O	1:A:1030:ARG:HB2	1.89	0.70
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.25	0.70
1:C:115:MET:CE	1:C:118:LEU:HD23	2.20	0.70
1:C:552:MET:SD	1:C:909:VAL:HG23	2.30	0.70
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.72	0.70
1:A:713:LEU:CG	1:A:833:PRO:HD3	2.20	0.70
1:C:202:ASP:OD2	1:C:792:ARG:NH2	2.25	0.70
1:C:527:TYR:OH	1:C:968:VAL:HG12	1.91	0.70
1:A:1033:PHE:O	1:A:1034:SER:HB2	1.91	0.70
1:B:5:PHE:HE2	1:B:11:PHE:HD2	1.40	0.70
1:A:400:LEU:HD11	1:A:930:GLY:HA2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:VAL:HG11	1:C:405:LEU:HD22	1.74	0.70
1:A:818:ARG:HA	1:A:824:SER:H	1.57	0.70
1:B:347:ALA:HB1	1:B:402:ILE:HG21	1.72	0.70
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.27	0.70
1:A:389:SER:O	1:A:394:THR:HG21	1.92	0.70
1:A:407:ASP:OD2	1:A:978:THR:HG21	1.91	0.69
1:B:727:PHE:HE1	1:B:786:ILE:HD11	1.57	0.69
1:C:465:ALA:O	1:C:469:GLN:HG2	1.91	0.69
1:C:538:THR:HG22	1:C:539:GLY:H	1.56	0.69
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.07	0.69
1:B:332:PHE:CD1	1:B:569:GLN:HA	2.26	0.69
1:C:491:ALA:C	1:C:493:CYS:H	2.00	0.69
1:C:417:GLU:OE2	1:C:417:GLU:HA	1.90	0.69
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.73	0.69
1:B:459:PHE:O	1:B:464:GLY:HA3	1.92	0.69
1:C:950:LYS:HA	1:C:953:MET:CE	2.19	0.69
1:A:391:ASN:O	1:A:392:THR:C	2.36	0.69
1:C:332:PHE:CD2	1:C:569:GLN:HA	2.28	0.69
1:A:603:LYS:H	1:A:603:LYS:HD3	1.58	0.69
1:B:412:VAL:HG13	1:B:435:MET:HE1	1.75	0.69
1:B:425:LEU:HB3	1:B:498:LYS:C	2.18	0.69
1:C:600:THR:O	1:C:603:LYS:HB2	1.92	0.69
1:A:69:MET:O	1:C:168:ARG:HG2	1.93	0.69
1:A:677:ALA:C	1:A:679:GLY:H	2.01	0.68
1:A:901:VAL:O	1:A:904:VAL:CG2	2.40	0.68
1:C:454:VAL:HG23	1:C:475:VAL:HG21	1.75	0.68
1:A:7:ASP:O	1:A:9:PRO:HD3	1.93	0.68
1:B:523:SER:HA	1:B:526:HIS:CD2	2.28	0.68
1:B:704:ALA:O	1:B:705:GLU:HB2	1.94	0.68
1:C:727:PHE:CE2	1:C:807:SER:HB2	2.27	0.68
1:C:190:PRO:HD2	1:C:779:TYR:HD1	1.54	0.68
1:C:418:ARG:HD2	1:C:419:VAL:HG22	1.74	0.68
1:B:393:LEU:HD13	1:B:466:ILE:HG23	1.74	0.68
1:C:445:ILE:HG13	1:C:446:ALA:H	1.57	0.68
1:C:476:SER:O	1:C:478:MET:N	2.25	0.68
1:A:818:ARG:HB3	1:A:823:PRO:HA	1.74	0.68
1:C:34:GLN:HB3	1:C:333:VAL:HG22	1.76	0.68
1:A:10:ILE:HG12	1:B:895:TRP:HB2	1.74	0.68
1:C:101:ASP:O	1:C:105:VAL:HG23	1.93	0.68
1:C:265:VAL:O	1:C:266:ALA:HB2	1.93	0.68
1:B:190:PRO:HD3	1:B:779:TYR:CE2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLY:O	1:A:388:PHE:O	2.12	0.68
1:B:648:THR:HG23	1:B:665:ALA:HB3	1.76	0.68
1:C:554:TYR:HB3	1:C:558:ARG:HH21	1.57	0.68
1:B:213:GLN:HB2	1:B:239:ARG:HD2	1.76	0.67
1:B:573:MET:HE2	1:B:676:THR:OG1	1.93	0.67
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.75	0.67
1:C:552:MET:SD	1:C:909:VAL:CG2	2.82	0.67
1:A:83:ASP:HB3	1:A:815:ARG:HG3	1.75	0.67
1:B:591:LEU:HD12	1:B:611:ALA:HB1	1.76	0.67
1:B:252:LYS:HB3	1:B:260:VAL:HG12	1.76	0.67
1:B:851:LEU:N	1:B:852:PRO:HD3	2.09	0.67
1:A:104:GLN:NE2	1:A:131:LYS:HD3	2.10	0.67
1:C:841:MET:HE1	1:C:866:GLU:HG3	1.76	0.67
1:B:20:MET:HG2	1:B:377:LEU:HD12	1.77	0.67
1:B:229:GLN:HA	1:C:583:THR:HG21	1.77	0.67
1:B:696:THR:HG22	1:B:699:ARG:HH12	1.60	0.67
1:C:190:PRO:CD	1:C:779:TYR:CD1	2.77	0.67
1:A:276:ASP:HB3	1:C:222:THR:HG23	1.76	0.67
1:A:188:MET:HA	1:A:266:ALA:HB2	1.76	0.66
1:A:560:PRO:HB2	1:A:922:THR:HG22	1.77	0.66
1:A:643:LYS:O	1:A:647:ILE:HG12	1.95	0.66
1:B:897:ILE:HB	1:B:1026:PHE:CE1	2.27	0.66
1:B:699:ARG:HG2	1:B:700:ASN:H	1.58	0.66
1:A:746:ILE:HD12	1:A:804:PHE:CE1	2.30	0.66
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.77	0.66
1:B:898:PRO:HA	1:B:901:VAL:HG23	1.77	0.66
1:B:1028:VAL:O	1:B:1032:ARG:HB2	1.96	0.66
1:A:340:VAL:HG13	1:A:399:VAL:CG2	2.25	0.66
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.77	0.66
1:B:692:HIS:HE1	1:B:723:ASP:OD1	1.78	0.66
1:A:842:GLU:O	1:A:846:GLN:HG3	1.95	0.66
1:C:189:ASN:ND2	1:C:191:ASN:H	1.93	0.66
1:A:298:ASN:HD22	1:A:301:ASP:H	1.43	0.66
1:B:727:PHE:CE1	1:B:786:ILE:HD11	2.31	0.66
1:A:108:GLN:CD	1:B:112:GLN:HG3	2.21	0.65
1:A:403:GLY:HA3	1:A:982:PHE:CZ	2.32	0.65
1:A:525:HIS:HA	1:A:528:THR:HG22	1.76	0.65
1:C:712:MET:O	1:C:713:LEU:HD22	1.96	0.65
1:A:685:ILE:HG22	1:A:686:ASP:H	1.62	0.65
1:B:729:ILE:HG13	1:B:730:ASP:N	2.07	0.65
1:B:714:THR:CG2	1:B:830:GLN:HG3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ILE:HG13	1:C:446:ALA:N	2.11	0.65
1:C:945:ILE:HG13	1:C:946:VAL:H	1.62	0.65
1:B:404:LEU:HD13	1:B:449:LEU:HD21	1.78	0.65
1:C:489:THR:O	1:C:493:CYS:HB2	1.96	0.65
1:B:539:GLY:C	1:B:541:TYR:H	2.05	0.65
1:C:174:ASP:HB3	1:C:292:LYS:HB2	1.78	0.65
1:A:149:MET:HE3	1:A:154:ILE:HG12	1.78	0.65
1:A:597:TYR:CD1	1:A:597:TYR:C	2.74	0.65
1:A:178:PHE:HB2	1:A:288:GLY:N	2.11	0.65
1:B:255:GLN:HG3	1:B:256:ASP:H	1.61	0.65
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.32	0.65
1:C:252:LYS:HG2	1:C:260:VAL:HG12	1.79	0.65
1:C:34:GLN:HB3	1:C:333:VAL:HG21	1.79	0.64
1:A:601:LYS:O	1:A:602:GLU:HG2	1.98	0.64
1:C:1018:ALA:O	1:C:1022:VAL:HG12	1.96	0.64
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.79	0.64
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.28	0.64
1:A:441:ALA:O	1:A:445:ILE:HG23	1.97	0.64
1:B:1027:VAL:O	1:B:1031:ARG:HB3	1.97	0.64
1:A:911:GLY:HA2	1:A:914:LEU:HB2	1.79	0.64
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.78	0.64
1:A:729:ILE:CG2	1:A:730:ASP:N	2.60	0.64
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.79	0.64
1:B:459:PHE:CZ	1:B:876:LEU:HG	2.28	0.64
1:C:815:ARG:HG2	1:C:815:ARG:HH11	1.62	0.64
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.80	0.64
1:C:213:GLN:NE2	1:C:238:THR:HA	2.13	0.64
1:C:729:ILE:CD1	1:C:786:ILE:HD13	2.27	0.64
1:A:14:VAL:O	1:A:17:ILE:N	2.31	0.64
1:B:36:PRO:O	1:B:38:ILE:HG12	1.98	0.64
1:C:158:VAL:CG1	1:C:177:LEU:HD21	2.28	0.64
1:A:117:LEU:HD11	1:C:124:GLN:O	1.97	0.63
1:A:836:SER:OG	1:A:839:GLU:HG2	1.98	0.63
1:B:792:ARG:HG2	1:B:793:ALA:H	1.63	0.63
1:A:328:ASP:OD1	1:A:330:THR:HB	1.98	0.63
1:C:102:ILE:HA	1:C:105:VAL:HG23	1.79	0.63
1:A:9:PRO:HD2	1:B:893:GLU:OE2	1.98	0.63
1:B:104:GLN:C	1:B:104:GLN:NE2	2.56	0.63
1:B:298:ASN:HB2	1:B:301:ASP:HB2	1.79	0.63
1:C:832:ALA:HB1	1:C:833:PRO:CD	2.29	0.63
1:A:886:LEU:HG	1:C:14:VAL:CG2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ARG:NH2	1:C:970:MET:CE	2.60	0.63
1:A:166:ILE:HD11	1:A:310:LEU:HD21	1.78	0.63
1:A:351:VAL:HG12	1:A:351:VAL:O	1.98	0.63
1:A:367:ILE:HG22	1:A:496:MET:CE	2.29	0.63
1:C:53:ASP:OD1	1:C:56:THR:HB	1.99	0.63
1:B:72:ILE:N	1:B:72:ILE:HD13	2.14	0.63
1:B:706:ALA:HB1	1:B:716:VAL:HG21	1.80	0.63
1:B:2:PRO:HB3	1:B:486:LEU:O	1.99	0.62
1:A:351:VAL:HG21	1:A:406:VAL:HG21	1.81	0.62
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.81	0.62
1:A:837:THR:HG22	1:A:841:MET:HE3	1.81	0.62
1:A:968:VAL:HG21	1:A:1023:PRO:HB3	1.80	0.62
1:A:354:VAL:HG11	1:A:980:LEU:HB3	1.81	0.62
1:A:713:LEU:O	1:A:714:THR:HG23	1.99	0.62
1:B:281:PHE:HE1	1:B:608:SER:HB2	1.62	0.62
1:B:444:GLY:HA2	1:B:891:LEU:HD11	1.81	0.62
1:B:667:ASN:O	1:B:678:THR:HB	1.99	0.62
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.34	0.62
1:A:702:LEU:HB2	1:A:851:LEU:HD11	1.81	0.62
1:B:228:GLN:NE2	1:C:781:MET:HB3	2.14	0.62
1:B:966:ASP:O	1:B:970:MET:HG3	1.98	0.62
1:A:894:SER:OG	1:A:897:ILE:HB	1.99	0.62
1:B:94:PHE:CB	1:B:98:THR:HG21	2.30	0.62
1:B:274:ASN:HD22	1:B:276:ASP:HB2	1.64	0.62
1:B:671:ILE:CG2	1:B:672:VAL:H	2.12	0.62
1:C:974:PRO:HA	1:C:977:MET:CE	2.28	0.62
1:A:139:VAL:CG1	1:A:327:TYR:HB3	2.27	0.62
1:C:15:ILE:O	1:C:19:ILE:HG12	1.99	0.62
1:C:222:THR:HG22	1:C:223:PRO:HD3	1.81	0.62
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.81	0.62
1:A:773:VAL:CG1	1:A:773:VAL:O	2.47	0.62
1:B:198:LEU:HD23	1:B:792:ARG:NH2	2.15	0.62
1:C:189:ASN:C	1:C:189:ASN:ND2	2.58	0.62
1:C:361:ASN:HB2	1:C:364:ALA:HB3	1.82	0.62
1:C:836:SER:HB3	1:C:839:GLU:HG2	1.82	0.62
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.30	0.62
1:B:158:VAL:HA	1:B:162:MET:HG3	1.81	0.62
1:B:255:GLN:HG3	1:B:256:ASP:N	2.14	0.62
1:B:255:GLN:CG	1:B:256:ASP:H	2.12	0.62
1:A:228:GLN:OE1	1:B:781:MET:HE3	2.00	0.61
1:B:14:VAL:HG11	1:C:890:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLY:HA3	1:C:377:LEU:O	1.99	0.61
1:C:695:LEU:HD13	1:C:825:MET:HE3	1.82	0.61
1:B:671:ILE:HG22	1:B:672:VAL:H	1.65	0.61
1:C:343:THR:O	1:C:343:THR:HG22	1.99	0.61
1:C:990:VAL:HG13	1:C:1005:THR:HG22	1.82	0.61
1:B:5:PHE:HE2	1:B:11:PHE:CD2	2.18	0.61
1:C:414:GLU:HB2	1:C:977:MET:HE1	1.82	0.61
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.35	0.61
1:B:671:ILE:CG2	1:B:672:VAL:N	2.63	0.61
1:C:945:ILE:HG13	1:C:946:VAL:N	2.16	0.61
1:A:993:THR:HG21	1:A:1000:GLN:OE1	2.00	0.61
1:B:712:MET:HE3	1:B:712:MET:HA	1.83	0.61
1:A:246:PHE:O	1:A:249:ILE:HG12	2.01	0.61
1:A:883:VAL:O	1:A:887:CYS:HB2	2.00	0.61
1:A:339:GLU:O	1:A:341:VAL:N	2.33	0.61
1:A:375:VAL:HG21	1:A:481:SER:HA	1.81	0.61
1:B:743:ILE:H	1:B:743:ILE:CD1	2.09	0.61
1:A:354:VAL:O	1:A:354:VAL:HG12	2.00	0.61
1:A:73:ASP:N	1:A:106:GLN:HE22	1.92	0.61
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.36	0.61
1:C:228:GLN:HG3	1:C:229:GLN:O	2.01	0.61
1:A:228:GLN:HG3	1:A:229:GLN:N	2.15	0.61
1:B:898:PRO:C	1:B:900:SER:N	2.59	0.61
1:C:1:MET:HB2	1:C:2:PRO:HD3	1.82	0.61
1:C:355:MET:HE3	1:C:355:MET:HA	1.81	0.61
1:A:485:ALA:HA	1:A:489:THR:OG1	2.02	0.60
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.31	0.60
1:C:38:ILE:CD1	1:C:38:ILE:N	2.64	0.60
1:A:344:LEU:HD23	1:A:402:ILE:HD12	1.82	0.60
1:B:68:ASN:HD22	1:B:114:ALA:HB2	1.66	0.60
1:C:686:ASP:OD1	1:C:686:ASP:C	2.44	0.60
1:A:660:ASP:O	1:A:661:ALA:HB2	2.00	0.60
1:B:119:PRO:C	1:B:121:GLU:H	2.09	0.60
1:A:355:MET:HE1	1:A:413:VAL:HG11	1.83	0.60
1:A:597:TYR:O	1:A:601:LYS:HB3	2.02	0.60
1:B:204:ILE:CG2	1:B:208:LYS:HE2	2.30	0.60
1:B:274:ASN:ND2	1:B:276:ASP:HB2	2.16	0.60
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.84	0.60
1:B:983:ILE:HD13	1:B:1012:VAL:HG12	1.83	0.60
1:C:38:ILE:HD13	1:C:38:ILE:N	2.15	0.60
1:A:293:LEU:O	1:A:294:ALA:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ALA:O	1:A:663:VAL:HG23	2.02	0.60
1:C:836:SER:HB3	1:C:839:GLU:CG	2.31	0.60
1:A:224:PRO:HB2	1:B:781:MET:HE1	1.84	0.60
1:A:353:LEU:C	1:A:355:MET:H	2.09	0.60
1:A:993:THR:HB	1:A:997:SER:CB	2.32	0.60
1:C:379:THR:HB	1:C:398:MET:CE	2.31	0.60
1:B:282:ASN:O	1:B:284:GLN:N	2.34	0.60
1:B:665:ALA:O	1:B:666:PHE:HB2	2.01	0.60
1:C:973:ARG:N	1:C:974:PRO:HD2	2.17	0.60
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.82	0.60
1:B:146:ASP:O	1:B:148:THR:N	2.32	0.60
1:C:310:LEU:HD13	1:C:323:ILE:HD13	1.83	0.60
1:C:767:ARG:HD3	1:C:769:LYS:HE3	1.81	0.60
1:B:10:ILE:HG13	1:C:893:GLU:O	2.02	0.59
1:B:30:LEU:HD13	1:B:390:ILE:HD11	1.83	0.59
1:C:40:PRO:HB2	1:C:94:PHE:O	2.02	0.59
1:C:762:PHE:CE1	1:C:769:LYS:HB2	2.37	0.59
1:B:476:SER:O	1:B:480:LEU:HB2	2.03	0.59
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.84	0.59
1:C:601:LYS:C	1:C:603:LYS:H	2.10	0.59
1:C:945:ILE:HD11	1:C:1022:VAL:HG22	1.84	0.59
1:B:151:GLN:O	1:B:155:SER:HB2	2.02	0.59
1:B:258:SER:C	1:B:259:ARG:HG2	2.28	0.59
1:B:193:LEU:HD22	1:B:198:LEU:HB2	1.83	0.59
1:C:795:ASP:OD2	1:C:797:GLN:HB3	2.02	0.59
1:C:948:PHE:HE1	1:C:971:ARG:HE	1.48	0.59
1:A:685:ILE:HG22	1:A:686:ASP:N	2.18	0.59
1:A:781:MET:HE3	1:C:228:GLN:CD	2.27	0.59
1:B:276:ASP:O	1:B:614:GLY:HA3	2.02	0.59
1:B:552:MET:SD	1:B:909:VAL:HG23	2.43	0.59
1:C:220:GLY:HA3	1:C:231:ASN:HD22	1.68	0.59
1:C:456:MET:HE3	1:C:932:LEU:HD12	1.83	0.59
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.83	0.59
1:C:958:LYS:HG2	1:C:962:GLU:HB3	1.85	0.59
1:A:254:ASN:ND2	1:A:258:SER:OG	2.36	0.59
1:A:841:MET:HE1	1:A:866:GLU:HG2	1.84	0.59
1:A:919:ARG:HG3	1:A:920:GLY:N	2.16	0.59
1:C:1:MET:CB	1:C:2:PRO:CD	2.80	0.59
1:C:466:ILE:HG13	1:C:563:PHE:HZ	1.65	0.59
1:A:612:VAL:HG22	1:A:626:ILE:HG22	1.83	0.59
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1017:LEU:O	1:C:1021:PHE:HB2	2.03	0.59
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.84	0.59
1:A:649:MET:O	1:A:653:ARG:HD3	2.02	0.59
1:A:680:PHE:CE1	1:A:829:GLY:HA3	2.38	0.59
1:B:418:ARG:HB3	1:B:418:ARG:HH11	1.66	0.59
1:B:876:LEU:CD2	1:B:932:LEU:HD11	2.32	0.59
1:C:435:MET:HE2	1:C:490:PRO:HB3	1.85	0.59
1:C:759:VAL:HB	1:C:760:ASN:ND2	2.17	0.59
1:A:169:THR:HG22	1:A:309:GLU:HG3	1.85	0.59
1:A:671:ILE:HD13	1:A:671:ILE:N	2.15	0.59
1:B:375:VAL:HG13	1:B:480:LEU:HB3	1.85	0.59
1:B:541:TYR:C	1:B:543:VAL:H	2.11	0.59
1:B:876:LEU:HD22	1:B:932:LEU:HD11	1.85	0.59
1:B:910:ILE:HG23	1:B:911:GLY:H	1.67	0.59
1:C:38:ILE:H	1:C:38:ILE:CD1	2.16	0.59
1:C:44:THR:CG2	1:C:91:THR:HB	2.22	0.59
1:A:225:VAL:HG12	1:B:781:MET:HE2	1.83	0.58
1:A:448:VAL:HG22	1:A:884:VAL:HG13	1.85	0.58
1:B:169:THR:O	1:B:172:VAL:HG23	2.02	0.58
1:A:239:ARG:HD3	1:A:762:PHE:HA	1.85	0.58
1:A:919:ARG:HG3	1:A:920:GLY:H	1.69	0.58
1:A:987:MET:N	1:A:988:PRO:CD	2.66	0.58
1:B:99:ASP:C	1:B:99:ASP:OD2	2.46	0.58
1:B:240:LEU:O	1:B:762:PHE:HB2	2.03	0.58
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.85	0.58
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.85	0.58
1:A:671:ILE:HG12	1:A:674:LEU:HB3	1.85	0.58
1:B:119:PRO:HG2	1:B:122:VAL:CG2	2.34	0.58
1:B:449:LEU:HB3	1:B:478:MET:HG3	1.85	0.58
1:C:474:ILE:O	1:C:478:MET:HB2	2.03	0.58
1:C:997:SER:O	1:C:999:ALA:N	2.36	0.58
1:A:293:LEU:O	1:A:294:ALA:HB2	2.03	0.58
1:B:782:LEU:N	1:B:785:ASP:OD1	2.36	0.58
1:B:70:ASN:HD22	1:B:70:ASN:N	1.99	0.58
1:B:518:ARG:HA	1:B:521:GLU:CD	2.28	0.58
1:B:967:ALA:C	1:B:969:ARG:N	2.61	0.58
1:A:216:ALA:CB	1:B:750:LEU:HD13	2.33	0.58
1:B:183:ALA:N	1:B:271:GLY:O	2.36	0.58
1:B:213:GLN:CG	1:C:56:THR:OG1	2.51	0.58
1:B:525:HIS:HA	1:B:528:THR:HG22	1.86	0.58
1:B:552:MET:C	1:B:554:TYR:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1022:VAL:HA	1:C:1025:PHE:CD2	2.39	0.58
1:A:401:ALA:HB2	1:A:474:ILE:HG13	1.85	0.58
1:B:888:LEU:C	1:B:890:ALA:H	2.11	0.58
1:B:70:ASN:H	1:B:70:ASN:ND2	2.01	0.58
1:C:412:VAL:HG12	1:C:412:VAL:O	2.04	0.58
1:C:16:ALA:O	1:C:20:MET:HG3	2.04	0.58
1:C:355:MET:HB3	1:C:365:THR:HG23	1.86	0.58
1:A:688:ALA:O	1:A:690:LEU:N	2.37	0.58
1:A:713:LEU:HB3	1:A:832:ALA:CB	2.34	0.58
1:B:537:SER:HB2	1:B:540:ARG:HE	1.68	0.58
1:B:593:GLU:OE2	1:B:658:ILE:HD13	2.04	0.58
1:B:911:GLY:HA3	1:B:1013:THR:HB	1.86	0.58
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.18	0.58
1:C:158:VAL:HG11	1:C:177:LEU:HD21	1.86	0.58
1:C:577:GLN:HA	1:C:577:GLN:HE21	1.68	0.58
1:A:154:ILE:O	1:A:158:VAL:HG23	2.04	0.57
1:A:634:TRP:H	1:A:634:TRP:CD1	2.21	0.57
1:A:688:ALA:C	1:A:690:LEU:H	2.12	0.57
1:B:201:VAL:HG21	1:B:745:ASP:OD1	2.03	0.57
1:B:948:PHE:HB2	1:B:971:ARG:NH2	2.19	0.57
1:A:359:LEU:HD13	1:A:977:MET:HE1	1.86	0.57
1:B:282:ASN:C	1:B:284:GLN:H	2.12	0.57
1:C:84:SER:HB2	1:C:814:PRO:HA	1.86	0.57
1:A:671:ILE:HG12	1:A:674:LEU:HD12	1.85	0.57
1:A:729:ILE:HD13	1:C:234:ILE:HG23	1.85	0.57
1:A:742:SER:OG	1:A:745:ASP:HB2	2.05	0.57
1:C:945:ILE:HG22	1:C:971:ARG:HB2	1.86	0.57
1:B:973:ARG:HG2	1:B:977:MET:HE2	1.86	0.57
1:C:197:GLN:HA	1:C:798:MET:HE2	1.85	0.57
1:A:340:VAL:HG13	1:A:399:VAL:HG23	1.85	0.57
1:A:731:ILE:CG1	1:A:746:ILE:HG21	2.30	0.57
1:B:605:ASN:HD21	1:B:642:ASN:ND2	2.01	0.57
1:C:531:VAL:O	1:C:534:ILE:HG12	2.04	0.57
1:C:746:ILE:HD12	1:C:804:PHE:CE1	2.39	0.57
1:C:972:LEU:H	1:C:974:PRO:HD2	1.69	0.57
1:C:327:TYR:HB2	1:C:628:PHE:HB3	1.85	0.57
1:A:225:VAL:H	1:B:781:MET:CE	2.18	0.57
1:A:979:SER:OG	1:A:1015:THR:HG21	2.05	0.57
1:B:742:SER:OG	1:B:745:ASP:HB2	2.05	0.57
1:C:329:THR:C	1:C:331:PRO:HD2	2.30	0.57
1:C:963:ALA:C	1:C:965:LEU:H	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HG2	1:A:129:VAL:HB	1.86	0.57
1:A:773:VAL:O	1:A:773:VAL:HG12	2.04	0.57
1:B:49:TYR:CE1	1:B:60:THR:HG21	2.40	0.57
1:B:633:ASP:OD1	1:B:634:TRP:N	2.36	0.57
1:B:967:ALA:C	1:B:969:ARG:H	2.12	0.57
1:C:580:ALA:HA	1:C:623:ASN:ND2	2.20	0.57
1:C:935:ILE:HG22	1:C:935:ILE:O	2.05	0.57
1:A:365:THR:O	1:A:368:PRO:HD2	2.05	0.56
1:A:712:MET:SD	1:A:835:LYS:HG2	2.45	0.56
1:C:110:LYS:O	1:C:111:LEU:C	2.47	0.56
1:A:713:LEU:CG	1:A:832:ALA:HA	2.34	0.56
1:B:204:ILE:HG22	1:B:208:LYS:HE2	1.86	0.56
1:B:356:TYR:O	1:B:360:GLN:N	2.37	0.56
1:C:331:PRO:O	1:C:335:ILE:HG12	2.05	0.56
1:B:187:TRP:O	1:B:266:ALA:HB1	2.04	0.56
1:B:911:GLY:HA3	1:B:1013:THR:CB	2.35	0.56
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.40	0.56
1:C:568:ASP:HB2	1:C:643:LYS:HG3	1.88	0.56
1:A:324:VAL:HG12	1:A:325:TYR:H	1.71	0.56
1:A:563:PHE:O	1:A:564:LEU:HD12	2.05	0.56
1:A:780:ARG:HH22	1:C:223:PRO:HD2	1.69	0.56
1:A:901:VAL:HG11	1:A:943:ILE:HG13	1.88	0.56
1:B:785:ASP:O	1:B:786:ILE:C	2.49	0.56
1:A:30:LEU:HD21	1:A:384:ALA:CB	2.27	0.56
1:A:746:ILE:HG22	1:A:747:ASN:N	2.19	0.56
1:B:192:GLU:O	1:B:196:PHE:HD2	1.89	0.56
1:B:225:VAL:HG23	1:C:781:MET:SD	2.46	0.56
1:A:756:GLY:HA2	1:A:774:MET:CB	2.36	0.56
1:A:780:ARG:NH2	1:C:223:PRO:HD2	2.19	0.56
1:A:813:SER:HB3	1:A:816:LEU:HD21	1.88	0.56
1:A:1015:THR:C	1:A:1017:LEU:H	2.13	0.56
1:A:1015:THR:O	1:A:1017:LEU:N	2.34	0.56
1:B:238:THR:HG23	1:B:239:ARG:N	2.20	0.56
1:C:342:LYS:C	1:C:344:LEU:H	2.13	0.56
1:A:298:ASN:O	1:A:302:THR:HG23	2.05	0.56
1:C:911:GLY:HA3	1:C:1013:THR:CG2	2.36	0.56
1:A:281:PHE:O	1:A:282:ASN:C	2.47	0.56
1:A:449:LEU:O	1:A:453:PHE:HD1	1.89	0.56
1:A:740:GLY:HA3	1:A:794:ALA:H	1.71	0.56
1:B:159:ALA:HB1	1:B:181:GLN:HG3	1.87	0.56
1:B:790:TYR:CD1	1:B:800:PRO:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ASN:C	1:C:5:PHE:H	2.14	0.56
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.88	0.56
1:A:189:ASN:CG	1:A:192:GLU:HB2	2.31	0.56
1:A:740:GLY:HA3	1:A:794:ALA:CB	2.36	0.56
1:B:188:MET:HA	1:B:266:ALA:HB2	1.88	0.56
1:B:947:GLU:O	1:B:951:ASP:HB2	2.06	0.56
1:C:247:GLY:HA3	1:C:263:ARG:CZ	2.36	0.56
1:C:909:VAL:CG1	1:C:935:ILE:HD11	2.36	0.56
1:A:180:SER:O	1:A:181:GLN:HB2	2.05	0.56
1:A:534:ILE:O	1:A:534:ILE:HG13	2.06	0.56
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.88	0.56
1:B:314:GLU:N	1:B:315:PRO:CD	2.69	0.56
1:B:1020:PHE:O	1:B:1021:PHE:CB	2.48	0.56
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.20	0.55
1:B:57:VAL:HG23	1:B:82:SER:HB2	1.87	0.55
1:C:220:GLY:HA3	1:C:231:ASN:ND2	2.21	0.55
1:C:962:GLU:HA	1:C:965:LEU:HD13	1.87	0.55
1:B:897:ILE:O	1:B:900:SER:OG	2.18	0.55
1:A:225:VAL:H	1:B:781:MET:HE2	1.70	0.55
1:A:729:ILE:CG2	1:A:730:ASP:H	2.20	0.55
1:B:237:GLN:HG2	1:B:238:THR:N	2.21	0.55
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.86	0.55
1:C:5:PHE:HE2	1:C:11:PHE:HD2	1.54	0.55
1:C:225:VAL:O	1:C:226:LYS:C	2.48	0.55
1:B:139:VAL:O	1:B:140:VAL:C	2.49	0.55
1:C:183:ALA:HB1	1:C:770:LYS:O	2.07	0.55
1:A:986:VAL:O	1:A:986:VAL:HG13	2.06	0.55
1:B:4:PHE:O	1:B:5:PHE:HB2	2.07	0.55
1:B:600:THR:C	1:B:602:GLU:H	2.15	0.55
1:B:682:PHE:CE1	1:B:857:TYR:CD1	2.95	0.55
1:A:150:THR:N	1:A:153:ASP:OD2	2.35	0.55
1:A:167:SER:OG	1:A:175:VAL:CG2	2.55	0.55
1:A:184:MET:HG3	1:A:186:ILE:HD11	1.88	0.55
1:C:190:PRO:CD	1:C:779:TYR:HD1	2.17	0.55
1:B:900:SER:OG	1:B:1029:VAL:HG11	2.07	0.55
1:A:583:THR:CG2	1:A:584:GLN:N	2.70	0.55
1:B:24:GLY:HA2	1:B:27:ILE:HG23	1.89	0.55
1:C:111:LEU:HD11	1:C:115:MET:HE3	1.89	0.55
1:A:588:GLN:HG2	1:A:613:ASN:OD1	2.07	0.55
1:A:606:VAL:HA	1:A:631:LEU:HD23	1.89	0.55
1:A:713:LEU:HG	1:A:833:PRO:CD	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:ASP:HB3	1:B:806:SER:HB3	1.89	0.55
1:A:52:ALA:CB	1:A:57:VAL:HG23	2.36	0.55
1:A:686:ASP:OD1	1:A:686:ASP:C	2.50	0.55
1:A:726:GLN:NE2	1:C:235:ILE:HG13	2.22	0.55
1:B:5:PHE:CE2	1:B:11:PHE:HD2	2.23	0.55
1:B:166:ILE:C	1:B:168:ARG:H	2.14	0.55
1:B:375:VAL:HB	1:B:405:LEU:HD22	1.89	0.55
1:C:577:GLN:HB2	3:C:2002:RFP:H402	1.89	0.55
1:A:207:ILE:HB	1:A:759:VAL:HG11	1.89	0.54
1:A:733:GLN:OE1	1:A:743:ILE:CD1	2.56	0.54
1:B:452:VAL:O	1:B:453:PHE:HB2	2.07	0.54
1:C:680:PHE:HE1	1:C:844:MET:HE3	1.72	0.54
1:A:108:GLN:NE2	1:B:112:GLN:HG3	2.21	0.54
1:A:782:LEU:O	1:A:785:ASP:HB2	2.07	0.54
1:B:123:GLN:O	1:B:125:GLN:N	2.40	0.54
1:B:139:VAL:O	1:B:139:VAL:CG1	2.54	0.54
1:A:69:MET:HE2	1:A:107:VAL:HG13	1.90	0.54
1:A:102:ILE:O	1:A:106:GLN:HG3	2.08	0.54
1:A:531:VAL:HG12	1:A:535:LEU:HD11	1.89	0.54
1:B:686:ASP:HB2	1:B:695:LEU:HD23	1.89	0.54
1:B:239:ARG:NH2	1:B:761:ASP:HB2	2.21	0.54
1:B:1033:PHE:O	1:B:1034:SER:HB2	2.07	0.54
1:C:401:ALA:O	1:C:405:LEU:HG	2.08	0.54
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.42	0.54
1:A:880:SER:O	1:A:884:VAL:HG23	2.08	0.54
1:B:343:THR:HG21	1:B:1000:GLN:OE1	2.08	0.54
1:B:978:THR:HG22	1:B:979:SER:N	2.22	0.54
1:C:729:ILE:HD11	1:C:786:ILE:HD11	1.88	0.54
1:A:991:ILE:O	1:A:992:SER:CB	2.56	0.54
1:B:411:VAL:O	1:B:415:ASN:HB2	2.06	0.54
1:B:551:GLY:HA2	1:B:554:TYR:HB3	1.90	0.54
1:B:898:PRO:O	1:B:900:SER:N	2.40	0.54
1:C:265:VAL:O	1:C:265:VAL:HG23	2.06	0.54
1:C:365:THR:O	1:C:368:PRO:HD2	2.07	0.54
1:C:974:PRO:O	1:C:977:MET:HB2	2.08	0.54
1:A:315:PRO:O	1:A:316:PHE:HB2	2.08	0.54
1:A:750:LEU:O	1:A:754:TRP:HD1	1.90	0.54
1:B:255:GLN:CG	1:B:256:ASP:N	2.70	0.54
1:B:669:PRO:HB3	1:B:862:MET:HE2	1.89	0.54
1:B:948:PHE:HB2	1:B:971:ARG:CZ	2.37	0.54
1:C:144:ASN:HD21	1:C:148:THR:H	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:MET:HG3	1:C:664:PHE:CE1	2.43	0.54
1:B:84:SER:HB3	1:B:814:PRO:CA	2.33	0.54
1:C:325:TYR:N	1:C:325:TYR:CD1	2.76	0.54
1:B:792:ARG:HG2	1:B:793:ALA:N	2.22	0.53
1:B:952:LEU:HG	1:B:956:GLU:OE2	2.08	0.53
1:C:106:GLN:O	1:C:107:VAL:C	2.50	0.53
1:C:210:GLN:HE22	1:C:249:ILE:HA	1.73	0.53
1:C:265:VAL:O	1:C:266:ALA:CB	2.55	0.53
1:C:552:MET:O	1:C:554:TYR:N	2.41	0.53
1:A:360:GLN:HE22	1:A:517:ASN:HD21	1.56	0.53
1:B:335:ILE:HG13	1:B:634:TRP:CD1	2.43	0.53
1:C:211:ASN:ND2	1:C:240:LEU:HG	2.16	0.53
1:C:815:ARG:HG2	1:C:815:ARG:NH1	2.23	0.53
1:A:990:VAL:C	1:A:991:ILE:HG12	2.33	0.53
1:A:214:VAL:HG23	1:A:237:GLN:HB3	1.89	0.53
1:A:1029:VAL:HG12	1:A:1030:ARG:H	1.72	0.53
1:C:906:PRO:HA	1:C:909:VAL:HG22	1.91	0.53
1:A:38:ILE:HG12	1:A:674:LEU:HD23	1.89	0.53
1:A:617:PHE:O	1:A:619:GLY:N	2.42	0.53
1:B:351:VAL:HG12	1:B:351:VAL:O	2.08	0.53
1:B:559:LEU:HD23	1:B:560:PRO:HD2	1.91	0.53
1:B:598:TYR:HB3	1:B:606:VAL:HG11	1.90	0.53
1:C:153:ASP:OD2	1:C:182:TYR:OH	2.27	0.53
1:C:702:LEU:HB2	1:C:851:LEU:HD21	1.90	0.53
1:B:360:GLN:O	1:B:361:ASN:HB3	2.09	0.53
1:A:456:MET:O	1:A:458:PHE:N	2.42	0.53
1:B:188:MET:CE	1:B:203:VAL:HG21	2.37	0.53
1:B:894:SER:C	1:B:896:SER:H	2.16	0.53
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.90	0.53
1:C:162:MET:HA	1:C:313:MET:CE	2.32	0.53
1:C:732:ASP:O	1:C:733:GLN:C	2.51	0.53
1:B:419:VAL:HG12	1:B:419:VAL:O	2.09	0.53
1:C:692:HIS:CE1	1:C:721:LEU:HD21	2.43	0.53
1:C:907:LEU:HG	1:C:1017:LEU:HB3	1.91	0.53
1:A:574:THR:HG1	1:A:598:TYR:HE1	1.57	0.53
1:A:781:MET:HE3	1:C:228:GLN:OE1	2.08	0.53
1:B:699:ARG:HG2	1:B:700:ASN:N	2.24	0.53
1:B:878:ALA:O	1:B:882:ILE:HG12	2.09	0.53
1:C:139:VAL:HG12	1:C:326:PRO:HG2	1.90	0.53
1:C:176:GLN:HE22	1:C:620:ARG:NH1	2.07	0.53
1:A:8:ARG:HB3	1:B:893:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:THR:O	1:A:601:LYS:CB	2.57	0.53
1:B:420:MET:SD	1:B:424:GLY:HA2	2.49	0.53
1:A:211:ASN:CG	1:A:211:ASN:O	2.52	0.52
1:A:818:ARG:HA	1:A:824:SER:N	2.23	0.52
1:B:238:THR:CG2	1:B:239:ARG:N	2.71	0.52
1:C:552:MET:SD	1:C:909:VAL:HG21	2.49	0.52
1:A:902:MET:O	1:A:904:VAL:N	2.41	0.52
1:B:63:GLN:O	1:B:66:GLU:N	2.42	0.52
1:B:154:ILE:HG23	1:B:321:LEU:HD11	1.92	0.52
1:B:351:VAL:HA	1:B:354:VAL:HG22	1.91	0.52
1:C:314:GLU:HB2	1:C:315:PRO:HD3	1.91	0.52
1:C:847:LEU:HA	1:C:850:LYS:HG2	1.90	0.52
1:A:442:LEU:HA	1:A:445:ILE:HG13	1.92	0.52
1:B:20:MET:HG3	1:B:374:VAL:HA	1.90	0.52
1:C:66:GLU:O	1:C:69:MET:N	2.38	0.52
1:C:714:THR:HG23	1:C:830:GLN:O	2.08	0.52
1:B:185:ARG:HB2	1:B:269:GLU:O	2.10	0.52
1:A:688:ALA:C	1:A:690:LEU:N	2.68	0.52
1:C:2:PRO:O	1:C:6:ILE:N	2.42	0.52
1:A:451:ALA:O	1:A:453:PHE:N	2.42	0.52
1:A:781:MET:HE3	1:C:228:GLN:HB2	1.92	0.52
1:B:376:LEU:HD22	1:B:398:MET:HE2	1.92	0.52
1:C:115:MET:HE3	1:C:127:VAL:HG11	1.89	0.52
1:C:351:VAL:HG13	1:C:369:THR:HG22	1.91	0.52
1:A:909:VAL:CG1	1:A:913:LEU:HD22	2.40	0.52
1:B:881:LEU:O	1:B:882:ILE:C	2.53	0.52
1:C:280:GLU:HA	1:C:286:ALA:HB3	1.92	0.52
1:C:953:MET:SD	1:C:963:ALA:HB2	2.50	0.52
1:A:255:GLN:O	1:A:256:ASP:HB2	2.09	0.52
1:B:251:LEU:HB2	1:B:261:LEU:HA	1.92	0.52
1:B:565:PRO:HD3	1:B:924:ASP:OD1	2.09	0.52
1:A:459:PHE:O	1:A:460:GLY:O	2.27	0.52
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.92	0.52
1:C:1028:VAL:HA	1:C:1031:ARG:HB3	1.90	0.52
1:A:682:PHE:HE2	1:A:684:LEU:HD12	1.74	0.52
1:B:405:LEU:HD12	1:B:406:VAL:HG13	1.92	0.52
1:B:412:VAL:HG21	1:B:485:ALA:HB1	1.91	0.52
1:C:736:ALA:C	1:C:738:ALA:H	2.18	0.52
1:A:210:GLN:CG	1:A:249:ILE:HG23	2.27	0.51
1:A:993:THR:HB	1:A:997:SER:HB2	1.92	0.51
1:B:123:GLN:C	1:B:125:GLN:H	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:HD22	1:B:262:LEU:H	1.75	0.51
1:B:894:SER:CB	1:B:897:ILE:HG12	2.38	0.51
1:B:919:ARG:HD3	1:B:921:LEU:HD13	1.91	0.51
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.11	0.51
1:C:448:VAL:O	1:C:452:VAL:HG23	2.10	0.51
1:A:974:PRO:O	1:A:975:ILE:C	2.53	0.51
1:B:213:GLN:HG2	1:C:56:THR:OG1	2.10	0.51
1:B:692:HIS:CE1	1:B:723:ASP:OD1	2.60	0.51
1:C:3:ASN:OD1	1:C:432:ARG:HG3	2.10	0.51
1:C:305:ALA:O	1:C:306:ILE:C	2.53	0.51
1:C:580:ALA:HA	1:C:623:ASN:HD22	1.74	0.51
1:C:727:PHE:CE2	1:C:807:SER:CB	2.93	0.51
1:A:169:THR:CG2	1:A:309:GLU:HG3	2.40	0.51
1:A:902:MET:O	1:A:905:VAL:HG23	2.11	0.51
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.92	0.51
1:B:568:ASP:OD2	1:B:634:TRP:HH2	1.93	0.51
1:C:131:LYS:HB2	1:C:295:THR:HG21	1.93	0.51
1:A:703:LEU:HD11	1:A:718:PRO:HD3	1.93	0.51
1:B:530:SER:O	1:B:534:ILE:HG12	2.10	0.51
1:A:151:GLN:NE2	1:A:279:ALA:H	2.07	0.51
1:A:151:GLN:NE2	1:A:279:ALA:N	2.59	0.51
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.93	0.51
1:B:360:GLN:O	1:B:361:ASN:CB	2.59	0.51
1:A:265:VAL:O	1:A:265:VAL:CG1	2.58	0.51
1:B:518:ARG:HA	1:B:521:GLU:HB2	1.92	0.51
1:B:626:ILE:HD11	1:B:628:PHE:CZ	2.45	0.51
1:B:701:GLN:HB3	1:B:851:LEU:CD1	2.39	0.51
1:B:788:ASP:N	1:B:788:ASP:OD1	2.43	0.51
1:C:607:GLU:HB2	1:C:632:LYS:HG2	1.93	0.51
1:C:655:PHE:C	1:C:657:GLN:N	2.68	0.51
1:A:605:ASN:OD1	1:A:637:ARG:HG2	2.11	0.51
1:A:711:ASP:C	1:A:713:LEU:H	2.17	0.51
1:B:456:MET:HG3	1:B:467:TYR:CB	2.35	0.51
1:C:762:PHE:CZ	1:C:764:ASP:HB2	2.46	0.51
1:A:99:ASP:OD1	1:A:101:ASP:HB2	2.11	0.51
1:B:445:ILE:HG13	1:B:940:LYS:HG3	1.93	0.51
1:A:391:ASN:O	1:A:393:LEU:N	2.43	0.51
1:A:993:THR:HB	1:A:997:SER:HB3	1.92	0.51
1:B:654:ALA:C	1:B:656:SER:H	2.18	0.51
1:B:979:SER:HA	1:B:1011:MET:HE3	1.93	0.51
1:C:1028:VAL:HG12	1:C:1032:ARG:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:ND2	1:A:301:ASP:H	2.09	0.50
1:A:886:LEU:HD21	1:C:17:ILE:HG21	1.91	0.50
1:C:314:GLU:N	1:C:315:PRO:HD2	2.26	0.50
1:C:467:TYR:CZ	1:C:925:VAL:HG12	2.46	0.50
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.94	0.50
1:B:291:ILE:HD12	1:B:291:ILE:N	2.27	0.50
1:B:939:ALA:O	1:B:943:ILE:HG12	2.11	0.50
1:B:1027:VAL:O	1:B:1031:ARG:CB	2.59	0.50
1:C:144:ASN:ND2	1:C:148:THR:N	2.58	0.50
1:A:66:GLU:C	1:A:68:ASN:H	2.18	0.50
1:A:281:PHE:CZ	1:A:324:VAL:HG11	2.47	0.50
1:A:427:PRO:C	1:A:429:GLU:H	2.18	0.50
1:A:677:ALA:C	1:A:679:GLY:N	2.69	0.50
1:B:328:ASP:OD2	1:B:328:ASP:C	2.54	0.50
1:B:373:PRO:O	1:B:377:LEU:HG	2.11	0.50
1:C:190:PRO:HB3	1:C:789:TRP:CZ3	2.46	0.50
1:C:218:GLN:HE21	1:C:231:ASN:HD21	1.60	0.50
1:C:956:GLU:OE2	1:C:956:GLU:HA	2.11	0.50
1:A:456:MET:HB2	1:A:471:SER:HB2	1.94	0.50
1:A:909:VAL:HG12	1:A:913:LEU:HD22	1.93	0.50
1:B:1010:GLY:HA2	1:B:1013:THR:HG22	1.93	0.50
1:C:158:VAL:HG12	1:C:177:LEU:HD21	1.93	0.50
1:C:983:ILE:HD11	1:C:1011:MET:HB3	1.92	0.50
1:A:278:ILE:HB	1:A:613:ASN:HB3	1.92	0.50
1:A:591:LEU:HD12	1:A:613:ASN:HB2	1.94	0.50
1:A:728:LYS:NZ	1:C:236:ALA:O	2.45	0.50
1:A:888:LEU:HD11	1:A:943:ILE:HG12	1.94	0.50
1:C:513:PHE:CG	1:C:516:PHE:HB3	2.47	0.50
1:C:948:PHE:O	1:C:952:LEU:HB3	2.11	0.50
1:A:367:ILE:HG13	1:A:368:PRO:CD	2.41	0.50
1:A:671:ILE:CG1	1:A:674:LEU:HD12	2.41	0.50
1:C:156:ASP:O	1:C:157:TYR:C	2.55	0.50
1:C:470:PHE:CD2	1:C:929:VAL:HG11	2.47	0.50
1:A:456:MET:C	1:A:458:PHE:N	2.69	0.50
1:A:780:ARG:HH21	1:C:222:THR:H	1.58	0.50
1:B:493:CYS:O	1:B:497:LEU:CB	2.59	0.50
1:B:631:LEU:HD11	1:B:644:VAL:HG12	1.93	0.50
1:B:681:ASP:OD2	1:B:826:GLU:OE1	2.29	0.50
1:C:332:PHE:O	1:C:333:VAL:C	2.54	0.50
1:C:350:LEU:HD22	1:C:984:LEU:HB3	1.92	0.50
1:C:752:ALA:O	1:C:774:MET:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:SER:HB3	1:A:816:LEU:CD2	2.42	0.50
1:B:150:THR:HG23	1:B:153:ASP:OD1	2.11	0.50
1:B:338:HIS:HE1	1:B:342:LYS:HE3	1.76	0.50
1:C:220:GLY:HA2	1:C:228:GLN:HE21	1.77	0.50
1:C:456:MET:HE3	1:C:932:LEU:CD1	2.42	0.50
1:A:181:GLN:O	1:A:181:GLN:HG2	2.11	0.50
1:A:207:ILE:O	1:A:211:ASN:HB3	2.12	0.50
1:A:221:GLY:H	1:B:622:GLN:HE22	1.60	0.50
1:A:607:GLU:HB3	1:A:630:SER:O	2.12	0.50
1:B:103:ALA:O	1:B:107:VAL:HG23	2.12	0.50
1:B:149:MET:HG2	1:B:153:ASP:HB3	1.94	0.50
1:A:931:LEU:O	1:A:935:ILE:HG12	2.12	0.49
1:B:372:VAL:HG22	1:B:373:PRO:HD3	1.93	0.49
1:C:56:THR:O	1:C:60:THR:HB	2.12	0.49
1:C:291:ILE:HG21	1:C:306:ILE:CD1	2.42	0.49
1:C:914:LEU:O	1:C:915:ALA:HB3	2.11	0.49
1:A:317:PHE:HE2	1:A:323:ILE:HG23	1.77	0.49
1:B:104:GLN:HE21	1:B:105:VAL:N	2.10	0.49
1:B:213:GLN:HG3	1:C:56:THR:OG1	2.11	0.49
1:B:967:ALA:O	1:B:969:ARG:N	2.44	0.49
1:C:451:ALA:CB	1:C:883:VAL:HG12	2.42	0.49
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.74	0.49
1:C:908:GLY:CA	1:C:1014:ALA:HB2	2.39	0.49
1:C:911:GLY:HA3	1:C:1013:THR:CB	2.42	0.49
1:A:271:GLY:HA3	1:A:275:TYR:OH	2.12	0.49
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.95	0.49
1:B:221:GLY:HA3	1:C:780:ARG:NH1	2.28	0.49
1:B:420:MET:SD	1:B:425:LEU:N	2.77	0.49
1:B:462:SER:H	1:B:865:GLN:NE2	2.10	0.49
1:C:389:SER:O	1:C:394:THR:HG21	2.12	0.49
1:C:986:VAL:O	1:C:990:VAL:HG23	2.12	0.49
1:A:393:LEU:HD11	1:A:466:ILE:HG12	1.95	0.49
1:A:418:ARG:HD3	1:A:970:MET:HE2	1.93	0.49
1:A:623:ASN:O	1:A:623:ASN:CG	2.54	0.49
1:B:985:GLY:O	1:B:988:PRO:HD2	2.13	0.49
1:B:1018:ALA:O	1:B:1022:VAL:HG22	2.12	0.49
1:C:472:ILE:HG22	1:C:473:THR:N	2.25	0.49
1:C:680:PHE:CE1	1:C:844:MET:HE3	2.46	0.49
1:C:712:MET:C	1:C:713:LEU:HD22	2.37	0.49
1:C:805:SER:O	1:C:806:SER:HB3	2.13	0.49
1:C:1004:GLY:C	1:C:1006:GLY:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG12	1:A:215:ALA:N	2.28	0.49
1:A:228:GLN:HG3	1:A:229:GLN:H	1.77	0.49
1:A:235:ILE:HG22	1:A:235:ILE:O	2.13	0.49
1:A:890:ALA:HB2	1:C:14:VAL:HG11	1.94	0.49
1:B:3:ASN:HA	1:B:6:ILE:HD13	1.94	0.49
1:B:649:MET:O	1:B:653:ARG:HB2	2.11	0.49
1:B:906:PRO:HA	1:B:909:VAL:CG2	2.39	0.49
1:C:11:PHE:O	1:C:14:VAL:HG12	2.12	0.49
1:C:102:ILE:O	1:C:103:ALA:C	2.54	0.49
1:C:655:PHE:O	1:C:657:GLN:N	2.46	0.49
1:C:859:TRP:HB3	1:C:863:SER:O	2.12	0.49
1:A:435:MET:SD	1:A:490:PRO:HB3	2.52	0.49
1:B:182:TYR:O	1:B:769:LYS:HD2	2.13	0.49
1:B:291:ILE:N	1:B:291:ILE:CD1	2.76	0.49
1:C:636:ASP:N	1:C:636:ASP:OD2	2.44	0.49
1:A:38:ILE:N	1:A:38:ILE:HD13	2.28	0.49
1:A:746:ILE:CD1	1:A:804:PHE:CE1	2.96	0.49
1:A:888:LEU:HB3	1:A:898:PRO:HB3	1.95	0.49
1:B:119:PRO:HG2	1:B:122:VAL:HG23	1.95	0.49
1:B:332:PHE:HB2	1:B:569:GLN:O	2.12	0.49
1:C:131:LYS:HB2	1:C:295:THR:CG2	2.42	0.49
1:C:756:GLY:H	1:C:774:MET:HE3	1.78	0.49
1:A:167:SER:OG	1:A:175:VAL:HG22	2.13	0.49
1:A:223:PRO:HD3	1:B:275:TYR:HB2	1.95	0.49
1:B:539:GLY:H	1:B:540:ARG:NH2	2.10	0.49
1:B:561:SER:HA	1:B:923:ASN:HB3	1.95	0.49
1:C:186:ILE:HG13	1:C:268:ILE:CD1	2.42	0.49
1:A:323:ILE:HG12	1:A:325:TYR:HE1	1.78	0.49
1:A:447:MET:CB	1:A:887:CYS:SG	2.97	0.49
1:C:963:ALA:C	1:C:965:LEU:N	2.71	0.49
1:A:533:GLY:C	1:A:535:LEU:N	2.65	0.48
1:A:571:VAL:HG12	1:A:630:SER:HB3	1.94	0.48
1:A:578:LEU:HB3	1:A:579:PRO:CD	2.43	0.48
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.13	0.48
1:B:231:ASN:C	1:B:231:ASN:ND2	2.68	0.48
1:B:250:LEU:HA	1:B:261:LEU:HB3	1.94	0.48
1:B:539:GLY:C	1:B:541:TYR:N	2.71	0.48
1:A:102:ILE:HA	1:A:105:VAL:HG23	1.96	0.48
1:A:343:THR:HG21	1:A:399:VAL:HG13	1.94	0.48
1:B:193:LEU:HD23	1:B:265:VAL:HG21	1.95	0.48
1:B:401:ALA:O	1:B:405:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:LEU:O	1:B:935:ILE:HG12	2.13	0.48
1:C:844:MET:O	1:C:847:LEU:HD22	2.13	0.48
1:A:395:MET:HA	1:A:395:MET:CE	2.35	0.48
1:A:1011:MET:HA	1:A:1011:MET:CE	2.40	0.48
1:B:355:MET:HE3	1:B:369:THR:HG23	1.94	0.48
1:B:404:LEU:HD22	1:B:449:LEU:HD11	1.93	0.48
1:B:665:ALA:O	1:B:666:PHE:CB	2.61	0.48
1:B:749:THR:O	1:B:750:LEU:C	2.56	0.48
1:C:431:THR:O	1:C:435:MET:HG2	2.13	0.48
1:C:466:ILE:HG13	1:C:563:PHE:CZ	2.47	0.48
1:C:727:PHE:HE2	1:C:807:SER:CB	2.26	0.48
1:C:962:GLU:HA	1:C:965:LEU:HB2	1.95	0.48
1:A:579:PRO:O	1:A:580:ALA:C	2.55	0.48
1:B:34:GLN:O	1:B:391:ASN:HB2	2.13	0.48
1:B:404:LEU:HD21	1:B:937:LEU:HD21	1.95	0.48
1:B:963:ALA:HA	1:B:966:ASP:HB2	1.94	0.48
1:C:541:TYR:C	1:C:543:VAL:H	2.21	0.48
1:C:712:MET:CB	1:C:835:LYS:HG3	2.44	0.48
1:C:935:ILE:O	1:C:935:ILE:CG2	2.61	0.48
1:B:193:LEU:CD2	1:B:198:LEU:HB2	2.44	0.48
1:B:1022:VAL:HA	1:B:1025:PHE:CD1	2.48	0.48
1:C:192:GLU:HB3	1:C:265:VAL:HG12	1.96	0.48
1:C:244:GLU:O	1:C:263:ARG:NH2	2.46	0.48
1:A:178:PHE:HB2	1:A:288:GLY:CA	2.44	0.48
1:B:154:ILE:C	1:B:156:ASP:N	2.70	0.48
1:B:314:GLU:OE2	1:B:323:ILE:HD12	2.14	0.48
1:B:754:TRP:HH2	1:B:785:ASP:HB2	1.76	0.48
1:B:945:ILE:HG23	1:B:975:ILE:HD11	1.94	0.48
1:C:144:ASN:HD21	1:C:148:THR:N	2.12	0.48
1:C:194:ASN:O	1:C:195:LYS:C	2.57	0.48
1:C:211:ASN:ND2	1:C:240:LEU:H	2.12	0.48
1:C:229:GLN:O	1:C:230:LEU:HB3	2.13	0.48
1:C:230:LEU:C	1:C:230:LEU:HD13	2.39	0.48
1:C:463:THR:O	1:C:465:ALA:N	2.47	0.48
1:C:491:ALA:O	1:C:493:CYS:N	2.46	0.48
1:A:780:ARG:NH2	1:C:223:PRO:O	2.47	0.48
1:A:912:ALA:HB2	1:A:1010:GLY:HA3	1.95	0.48
1:B:44:THR:OG1	1:B:132:SER:HB3	2.13	0.48
1:B:158:VAL:HA	1:B:162:MET:HG2	1.93	0.48
1:B:314:GLU:HA	1:B:317:PHE:CE2	2.47	0.48
1:C:931:LEU:HD22	1:C:931:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ALA:C	1:A:453:PHE:H	2.20	0.48
1:A:923:ASN:C	1:A:923:ASN:HD22	2.22	0.48
1:B:200:PRO:HD2	1:B:749:THR:HG23	1.94	0.48
1:B:324:VAL:CG2	1:B:326:PRO:HD3	2.43	0.48
1:B:372:VAL:HB	1:B:405:LEU:HD11	1.96	0.48
1:B:408:ASP:OD1	1:B:442:LEU:HA	2.13	0.48
1:B:720:GLY:O	1:B:721:LEU:HD12	2.14	0.48
1:C:158:VAL:HG12	1:C:159:ALA:N	2.27	0.48
1:C:190:PRO:HB3	1:C:789:TRP:CE3	2.49	0.48
1:C:858:ASP:OD1	1:C:859:TRP:N	2.47	0.48
1:A:254:ASN:CG	1:A:258:SER:OG	2.57	0.48
1:A:729:ILE:HG22	1:A:730:ASP:H	1.76	0.48
1:B:200:PRO:HG2	1:B:749:THR:HG23	1.96	0.48
1:C:119:PRO:HG2	1:C:122:VAL:HG23	1.96	0.48
1:A:574:THR:HB	1:A:627:ALA:HB3	1.95	0.48
1:B:426:PRO:HB3	1:B:430:ALA:CB	2.44	0.48
1:B:655:PHE:O	1:B:658:ILE:HG13	2.13	0.48
1:B:990:VAL:HG21	1:B:1008:MET:SD	2.54	0.48
1:C:366:LEU:O	1:C:370:ILE:N	2.42	0.48
1:C:379:THR:CG2	1:C:477:ALA:HB2	2.44	0.48
1:C:948:PHE:HE1	1:C:971:ARG:NE	2.12	0.48
1:A:5:PHE:CD1	1:A:12:ALA:HB2	2.48	0.47
1:A:346:GLU:C	1:A:348:ILE:H	2.22	0.47
1:A:1033:PHE:O	1:A:1034:SER:CB	2.60	0.47
1:B:940:LYS:NZ	1:B:978:THR:CG2	2.77	0.47
1:A:527:TYR:CE2	1:A:972:LEU:HG	2.49	0.47
1:A:649:MET:HG2	1:A:653:ARG:NH1	2.29	0.47
1:A:897:ILE:N	1:A:898:PRO:HD2	2.29	0.47
1:A:987:MET:HA	1:A:990:VAL:O	2.14	0.47
1:B:157:TYR:HA	1:B:161:ASN:ND2	2.29	0.47
1:B:692:HIS:HE1	1:B:723:ASP:CG	2.22	0.47
1:B:762:PHE:HD2	1:B:771:VAL:HG22	1.78	0.47
1:B:940:LYS:HZ2	1:B:978:THR:CG2	2.28	0.47
1:B:1024:VAL:O	1:B:1028:VAL:HG23	2.14	0.47
1:C:294:ALA:HB3	1:C:297:ALA:HB2	1.96	0.47
1:C:909:VAL:HG11	1:C:935:ILE:HD11	1.96	0.47
1:C:973:ARG:O	1:C:977:MET:HG3	2.14	0.47
1:A:324:VAL:HG12	1:A:325:TYR:N	2.29	0.47
1:B:314:GLU:N	1:B:315:PRO:HD3	2.29	0.47
1:A:51:GLY:O	1:C:215:ALA:HB1	2.13	0.47
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:SER:HG	1:A:175:VAL:HG21	1.79	0.47
1:B:221:GLY:HA3	1:C:780:ARG:HH12	1.79	0.47
1:B:342:LYS:O	1:B:346:GLU:HG3	2.13	0.47
1:B:921:LEU:HD22	1:B:1005:THR:HB	1.97	0.47
1:C:3:ASN:C	1:C:5:PHE:N	2.71	0.47
1:C:18:ILE:O	1:C:19:ILE:C	2.58	0.47
1:A:674:LEU:HD13	1:A:675:GLY:N	2.29	0.47
1:A:818:ARG:NH1	1:A:821:GLY:O	2.47	0.47
1:A:991:ILE:O	1:A:992:SER:OG	2.26	0.47
1:B:210:GLN:NE2	1:B:249:ILE:HA	2.28	0.47
1:B:692:HIS:O	1:B:692:HIS:ND1	2.48	0.47
1:C:778:LYS:HG3	1:C:779:TYR:CE2	2.50	0.47
1:A:552:MET:HA	1:A:555:LEU:HB2	1.97	0.47
1:A:597:TYR:HD1	1:A:598:TYR:N	2.12	0.47
1:B:13:TRP:O	1:B:17:ILE:HG12	2.14	0.47
1:B:222:THR:CB	1:B:223:PRO:HD3	2.26	0.47
1:B:456:MET:CG	1:B:467:TYR:HB3	2.36	0.47
1:B:518:ARG:HA	1:B:521:GLU:CG	2.45	0.47
1:B:681:ASP:O	1:B:859:TRP:HE3	1.98	0.47
1:B:703:LEU:HA	1:B:706:ALA:HB3	1.96	0.47
1:C:713:LEU:HD23	1:C:832:ALA:N	2.29	0.47
1:A:210:GLN:HG3	1:A:249:ILE:CG2	2.29	0.47
1:A:314:GLU:O	1:A:317:PHE:HB2	2.15	0.47
1:A:337:ILE:HG12	1:A:395:MET:SD	2.54	0.47
1:A:568:ASP:CG	1:A:637:ARG:HH12	2.22	0.47
1:B:154:ILE:C	1:B:156:ASP:H	2.23	0.47
1:B:327:TYR:CD1	1:B:327:TYR:C	2.92	0.47
1:B:371:ALA:HA	1:B:374:VAL:HG12	1.96	0.47
1:B:666:PHE:HB3	1:B:678:THR:CG2	2.45	0.47
1:B:910:ILE:HG23	1:B:911:GLY:N	2.28	0.47
1:C:2:PRO:O	1:C:6:ILE:HG13	2.14	0.47
1:C:186:ILE:O	1:C:186:ILE:HG22	2.13	0.47
1:C:520:PHE:C	1:C:522:LYS:H	2.22	0.47
1:A:608:SER:O	1:A:629:VAL:HG23	2.15	0.47
1:A:1029:VAL:HG12	1:A:1030:ARG:N	2.30	0.47
1:B:549:VAL:O	1:B:552:MET:HB3	2.14	0.47
1:B:860:THR:O	1:B:863:SER:HB2	2.14	0.47
1:C:328:ASP:OD1	1:C:330:THR:HB	2.15	0.47
1:C:376:LEU:O	1:C:379:THR:N	2.44	0.47
1:C:457:ALA:HB2	1:C:471:SER:CB	2.45	0.47
1:C:491:ALA:C	1:C:493:CYS:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:926:TYR:CE2	1:C:999:ALA:HB1	2.50	0.47
1:C:949:ALA:HB1	1:C:1026:PHE:CE2	2.50	0.47
1:A:223:PRO:HD3	1:B:275:TYR:CD2	2.49	0.47
1:A:443:VAL:HG12	1:A:443:VAL:O	2.13	0.47
1:A:590:VAL:O	1:A:591:LEU:C	2.56	0.47
1:B:78:MET:HG3	1:B:92:LEU:HG	1.97	0.47
1:B:160:ALA:HB1	1:B:767:ARG:HD3	1.96	0.47
1:B:452:VAL:O	1:B:453:PHE:CB	2.63	0.47
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.78	0.47
1:C:497:LEU:HD12	1:C:498:LYS:HG3	1.96	0.47
1:A:150:THR:OG1	1:A:153:ASP:OD2	2.31	0.47
1:A:330:THR:O	1:A:331:PRO:C	2.58	0.47
1:A:351:VAL:HG21	1:A:406:VAL:CG2	2.45	0.47
1:A:431:THR:HB	1:A:494:ALA:HB2	1.95	0.47
1:A:673:GLU:O	1:A:673:GLU:HG3	2.15	0.47
1:A:808:ARG:N	1:A:808:ARG:HH11	2.12	0.47
1:B:997:SER:HA	1:B:1000:GLN:HB2	1.97	0.47
1:C:350:LEU:CD2	1:C:984:LEU:HB3	2.45	0.47
1:C:713:LEU:HD13	1:C:713:LEU:N	2.29	0.47
1:A:309:GLU:O	1:A:313:MET:HG2	2.15	0.46
1:A:681:ASP:H	1:A:863:SER:CB	2.28	0.46
1:B:115:MET:HB2	1:B:116:PRO:HD3	1.96	0.46
1:C:463:THR:HG22	1:C:464:GLY:N	2.29	0.46
1:A:346:GLU:C	1:A:348:ILE:N	2.71	0.46
1:A:445:ILE:HD12	1:A:445:ILE:C	2.40	0.46
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.97	0.46
1:A:1015:THR:C	1:A:1017:LEU:N	2.73	0.46
1:B:62:THR:O	1:B:66:GLU:HB2	2.14	0.46
1:B:72:ILE:HD13	1:B:72:ILE:H	1.79	0.46
1:B:469:GLN:O	1:B:473:THR:OG1	2.33	0.46
1:B:472:ILE:HG23	1:B:473:THR:N	2.30	0.46
1:B:908:GLY:C	1:B:910:ILE:H	2.23	0.46
1:C:484:VAL:HG13	1:C:488:LEU:HB3	1.98	0.46
1:C:778:LYS:HG3	1:C:779:TYR:HE2	1.81	0.46
1:C:821:GLY:O	1:C:822:LEU:HD23	2.15	0.46
1:C:966:ASP:O	1:C:970:MET:N	2.29	0.46
1:A:255:GLN:O	1:A:256:ASP:CB	2.63	0.46
1:A:367:ILE:HG12	1:A:413:VAL:HG21	1.97	0.46
1:A:545:TYR:HB2	1:A:1021:PHE:HE1	1.79	0.46
1:B:2:PRO:O	1:B:4:PHE:N	2.48	0.46
1:B:53:ASP:O	1:B:54:ALA:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLU:HG3	1:B:313:MET:HE3	1.96	0.46
1:C:899:PHE:HD1	1:C:899:PHE:H	1.62	0.46
1:A:281:PHE:O	1:A:283:GLY:N	2.48	0.46
1:A:995:ALA:O	1:A:996:GLY:C	2.59	0.46
1:C:371:ALA:HB2	1:C:488:LEU:HD23	1.97	0.46
1:C:655:PHE:O	1:C:656:SER:C	2.56	0.46
1:C:734:GLU:HA	1:C:737:GLN:HG2	1.97	0.46
1:C:1032:ARG:HG3	1:C:1036:LYS:HE2	1.97	0.46
1:A:973:ARG:O	1:A:977:MET:HG3	2.16	0.46
1:B:50:PRO:HG2	1:B:125:GLN:HE22	1.80	0.46
1:B:613:ASN:O	1:B:625:GLY:HA2	2.15	0.46
1:B:669:PRO:CB	1:B:862:MET:HE2	2.46	0.46
1:B:828:LEU:HB3	1:B:829:GLY:H	1.59	0.46
1:B:1009:GLY:O	1:B:1012:VAL:HG22	2.16	0.46
1:C:160:ALA:HA	1:C:767:ARG:NE	2.31	0.46
1:C:435:MET:HA	1:C:438:ILE:HG22	1.98	0.46
1:C:601:LYS:O	1:C:603:LYS:N	2.48	0.46
1:A:221:GLY:HA2	1:B:622:GLN:OE1	2.16	0.46
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.51	0.46
1:A:702:LEU:O	1:A:702:LEU:HG	2.16	0.46
1:B:111:LEU:HD21	1:B:127:VAL:HG13	1.97	0.46
1:B:445:ILE:O	1:B:449:LEU:HB2	2.16	0.46
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.98	0.46
1:C:658:ILE:HD12	1:C:658:ILE:H	1.81	0.46
1:A:274:ASN:OD1	1:A:275:TYR:N	2.49	0.46
1:C:317:PHE:CG	1:C:321:LEU:HD12	2.51	0.46
1:A:53:ASP:O	1:A:54:ALA:C	2.58	0.46
1:A:427:PRO:O	1:A:429:GLU:N	2.48	0.46
1:A:883:VAL:O	1:A:883:VAL:CG1	2.64	0.46
1:B:587:THR:HG22	1:B:591:LEU:HD23	1.98	0.46
1:C:379:THR:O	1:C:382:VAL:N	2.49	0.46
1:C:569:GLN:C	1:C:634:TRP:HZ2	2.24	0.46
1:C:767:ARG:HH11	1:C:767:ARG:HG3	1.81	0.46
1:C:911:GLY:CA	1:C:1013:THR:HG21	2.44	0.46
1:A:167:SER:OG	1:A:175:VAL:HG21	2.16	0.46
1:A:391:ASN:H	1:A:394:THR:HG22	1.80	0.46
1:B:671:ILE:HD13	1:B:676:THR:HG22	1.98	0.46
1:C:759:VAL:HG23	1:C:771:VAL:HB	1.98	0.46
1:C:997:SER:O	1:C:1000:GLN:N	2.41	0.46
1:A:133:SER:C	1:A:135:SER:H	2.23	0.45
1:A:729:ILE:HD13	1:C:234:ILE:CG2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:VAL:CG1	1:A:800:PRO:HD2	2.46	0.45
1:B:764:ASP:O	1:B:766:GLY:N	2.49	0.45
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.98	0.45
1:C:144:ASN:ND2	1:C:148:THR:H	2.14	0.45
1:C:531:VAL:HA	1:C:534:ILE:HG23	1.97	0.45
1:C:648:THR:O	1:C:649:MET:C	2.59	0.45
1:C:731:ILE:HG12	1:C:746:ILE:HG21	1.98	0.45
1:A:316:PHE:O	1:A:317:PHE:C	2.60	0.45
1:A:389:SER:OG	1:A:391:ASN:ND2	2.48	0.45
1:A:414:GLU:C	1:A:416:VAL:H	2.23	0.45
1:A:428:LYS:HG3	1:A:429:GLU:HG3	1.98	0.45
1:B:764:ASP:C	1:B:766:GLY:H	2.24	0.45
1:B:1022:VAL:HA	1:B:1025:PHE:HD1	1.80	0.45
1:C:457:ALA:HB2	1:C:471:SER:OG	2.17	0.45
1:A:56:THR:O	1:A:60:THR:HB	2.16	0.45
1:A:317:PHE:HE2	1:A:323:ILE:CG2	2.29	0.45
1:A:409:ALA:O	1:A:410:ILE:C	2.59	0.45
1:A:451:ALA:C	1:A:453:PHE:N	2.74	0.45
1:C:115:MET:HE2	1:C:115:MET:HA	1.97	0.45
1:A:431:THR:CB	1:A:494:ALA:HB2	2.46	0.45
1:A:530:SER:O	1:A:534:ILE:HG23	2.15	0.45
1:B:58:GLN:O	1:B:63:GLN:HG2	2.17	0.45
1:B:66:GLU:HG3	1:B:78:MET:SD	2.56	0.45
1:B:104:GLN:HE22	1:B:108:GLN:HE21	1.64	0.45
1:B:228:GLN:HE22	1:C:781:MET:HB3	1.79	0.45
1:B:399:VAL:O	1:B:402:ILE:HB	2.16	0.45
1:B:418:ARG:HB3	1:B:418:ARG:NH1	2.31	0.45
1:C:9:PRO:O	1:C:11:PHE:N	2.46	0.45
1:C:65:ILE:HD13	1:C:111:LEU:HD21	1.97	0.45
1:C:758:TYR:HE2	1:C:770:LYS:CB	2.18	0.45
1:B:541:TYR:C	1:B:543:VAL:N	2.75	0.45
1:C:345:VAL:O	1:C:348:ILE:N	2.48	0.45
1:C:693:GLU:O	1:C:694:LYS:C	2.60	0.45
1:A:60:THR:HG23	1:A:119:PRO:HG3	1.97	0.45
1:A:701:GLN:O	1:A:702:LEU:C	2.60	0.45
1:A:727:PHE:CZ	1:A:783:PRO:HB3	2.51	0.45
1:A:909:VAL:O	1:A:912:ALA:HB3	2.16	0.45
1:A:911:GLY:N	1:A:914:LEU:HD13	2.16	0.45
1:B:63:GLN:O	1:B:64:VAL:C	2.60	0.45
1:B:314:GLU:HG3	1:B:317:PHE:CE2	2.51	0.45
1:B:910:ILE:C	1:B:912:ALA:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:PHE:HA	1:C:369:THR:HG21	1.98	0.45
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.99	0.45
1:A:414:GLU:C	1:A:414:GLU:CD	2.85	0.45
1:A:680:PHE:CE1	1:A:844:MET:HE2	2.51	0.45
1:A:959:GLY:C	1:A:961:ILE:N	2.74	0.45
1:B:348:ILE:HG12	1:B:372:VAL:HG21	1.98	0.45
1:B:805:SER:O	1:B:806:SER:HB2	2.16	0.45
1:B:986:VAL:HG12	1:B:990:VAL:CG2	2.47	0.45
1:C:414:GLU:HG2	1:C:974:PRO:HB3	1.98	0.45
1:C:418:ARG:HD2	1:C:419:VAL:CG2	2.42	0.45
1:C:872:GLN:HE21	1:C:875:SER:HB2	1.81	0.45
1:C:901:VAL:HG11	1:C:943:ILE:HA	1.98	0.45
1:B:34:GLN:HG2	1:B:35:TYR:CD2	2.51	0.45
1:B:669:PRO:HG3	1:B:678:THR:HA	1.99	0.45
1:A:576:VAL:HG11	1:A:591:LEU:HD23	1.98	0.45
1:B:639:GLY:O	1:B:641:GLU:N	2.50	0.45
1:C:76:MET:HE2	1:C:94:PHE:O	2.17	0.45
1:C:155:SER:OG	1:C:179:GLY:HA3	2.17	0.45
1:A:747:ASN:O	1:A:748:THR:C	2.59	0.45
1:B:5:PHE:HA	1:B:8:ARG:HB2	1.99	0.45
1:B:44:THR:OG1	1:B:132:SER:CB	2.64	0.45
1:B:493:CYS:O	1:B:497:LEU:HB2	2.17	0.45
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.98	0.45
1:C:188:MET:HA	1:C:266:ALA:HB2	1.98	0.45
1:C:367:ILE:HG23	1:C:368:PRO:HD3	1.99	0.45
1:A:750:LEU:O	1:A:754:TRP:CD1	2.70	0.44
1:B:410:ILE:HD13	1:B:977:MET:HG3	1.99	0.44
1:B:891:LEU:HD13	1:B:892:TYR:CE2	2.52	0.44
1:C:925:VAL:HG23	1:C:926:TYR:N	2.32	0.44
1:A:69:MET:CG	1:A:92:LEU:HD21	2.48	0.44
1:A:83:ASP:O	1:A:85:THR:N	2.49	0.44
1:A:713:LEU:HB2	1:A:833:PRO:CD	2.36	0.44
1:A:923:ASN:C	1:A:923:ASN:ND2	2.75	0.44
1:B:261:LEU:O	1:B:263:ARG:N	2.50	0.44
1:B:291:ILE:CD1	1:B:291:ILE:H	2.30	0.44
1:B:601:LYS:HE2	1:B:601:LYS:HB2	1.90	0.44
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.46	0.44
1:C:314:GLU:N	1:C:315:PRO:CD	2.80	0.44
1:C:577:GLN:HE21	1:C:577:GLN:CA	2.25	0.44
1:A:241:THR:N	1:A:245:GLU:OE1	2.40	0.44
1:A:250:LEU:HD22	1:A:250:LEU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:ARG:O	1:A:974:PRO:HD2	2.17	0.44
1:B:157:TYR:C	1:B:161:ASN:HD22	2.24	0.44
1:B:225:VAL:O	1:B:226:LYS:C	2.60	0.44
1:B:238:THR:HG23	1:B:239:ARG:H	1.82	0.44
1:B:280:GLU:HA	1:B:286:ALA:HB3	1.99	0.44
1:B:339:GLU:O	1:B:342:LYS:HB2	2.16	0.44
1:C:713:LEU:HG	1:C:833:PRO:C	2.42	0.44
1:C:859:TRP:CE3	1:C:863:SER:HB3	2.53	0.44
1:A:353:LEU:C	1:A:355:MET:N	2.75	0.44
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.99	0.44
1:B:863:SER:O	1:B:866:GLU:N	2.50	0.44
1:B:891:LEU:HD13	1:B:892:TYR:CZ	2.52	0.44
1:B:892:TYR:CD1	1:B:897:ILE:HD11	2.51	0.44
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.99	0.44
1:C:219:LEU:CD2	1:C:234:ILE:HD11	2.47	0.44
1:A:359:LEU:O	1:A:360:GLN:HB2	2.17	0.44
1:A:540:ARG:HD2	1:A:541:TYR:CE2	2.52	0.44
1:A:574:THR:HG21	1:A:594:VAL:CG1	2.48	0.44
1:B:57:VAL:CG2	1:B:82:SER:HB2	2.47	0.44
1:B:60:THR:CG2	1:B:119:PRO:HG3	2.48	0.44
1:C:57:VAL:HG12	1:C:88:VAL:HG22	1.99	0.44
1:C:554:TYR:C	1:C:556:PHE:N	2.76	0.44
1:C:658:ILE:C	1:C:659:LYS:HD2	2.43	0.44
1:C:952:LEU:HG	1:C:952:LEU:O	2.18	0.44
1:A:190:PRO:HB3	1:A:789:TRP:CD2	2.52	0.44
1:A:471:SER:O	1:A:472:ILE:C	2.61	0.44
1:A:540:ARG:HD2	1:A:541:TYR:HE2	1.81	0.44
1:B:309:GLU:O	1:B:312:LYS:HB2	2.17	0.44
1:B:942:ALA:O	1:B:945:ILE:HG13	2.17	0.44
1:C:203:VAL:O	1:C:207:ILE:HG13	2.18	0.44
1:C:254:ASN:O	1:C:256:ASP:N	2.51	0.44
1:C:576:VAL:HG13	1:C:590:VAL:HG11	2.00	0.44
1:C:782:LEU:HB3	1:C:783:PRO:HD2	1.98	0.44
1:A:355:MET:CG	1:A:365:THR:HG22	2.48	0.44
1:A:877:TYR:OH	1:A:932:LEU:HD11	2.17	0.44
1:B:298:ASN:CB	1:B:301:ASP:HB2	2.47	0.44
1:B:563:PHE:HB2	1:B:866:GLU:HG3	1.98	0.44
1:C:390:ILE:HA	1:C:394:THR:HG21	1.99	0.44
1:C:657:GLN:O	1:C:659:LYS:N	2.51	0.44
1:A:591:LEU:CD1	1:A:613:ASN:HB2	2.48	0.44
1:A:724:THR:HG22	1:A:725:PRO:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:GLU:HB3	1:A:958:LYS:HG3	2.00	0.44
1:B:118:LEU:O	1:B:119:PRO:C	2.61	0.44
1:B:448:VAL:O	1:B:452:VAL:HG22	2.17	0.44
1:B:624:THR:O	1:B:624:THR:HG23	2.17	0.44
1:B:901:VAL:O	1:B:904:VAL:HG23	2.17	0.44
1:C:14:VAL:HG13	1:C:15:ILE:N	2.31	0.44
1:C:144:ASN:HA	1:C:320:GLY:O	2.16	0.44
1:C:267:LYS:HE3	1:C:267:LYS:HB2	1.87	0.44
1:C:759:VAL:C	1:C:760:ASN:HD22	2.25	0.44
1:C:928:GLN:HA	1:C:931:LEU:HB3	1.98	0.44
1:C:959:GLY:O	1:C:960:LEU:C	2.61	0.44
1:A:46:SER:HA	1:A:88:VAL:O	2.17	0.44
1:A:252:LYS:HE3	1:A:254:ASN:HB3	2.00	0.44
1:A:617:PHE:C	1:A:619:GLY:N	2.76	0.44
1:A:959:GLY:HA3	1:A:962:GLU:HB3	2.00	0.44
1:B:450:SER:O	1:B:452:VAL:O	2.36	0.44
1:B:560:PRO:HB2	1:B:836:SER:CB	2.41	0.44
1:C:574:THR:HG23	1:C:665:ALA:HB2	1.98	0.44
1:C:778:LYS:C	1:C:779:TYR:HD2	2.25	0.44
1:C:778:LYS:C	1:C:779:TYR:CD2	2.96	0.44
1:C:931:LEU:O	1:C:935:ILE:HG13	2.18	0.44
1:A:63:GLN:HG2	1:C:768:VAL:HG12	2.00	0.43
1:A:74:ASN:H	1:C:170:SER:HB2	1.83	0.43
1:A:733:GLN:HE22	1:A:743:ILE:HD12	1.83	0.43
1:A:780:ARG:NH2	1:C:222:THR:H	2.15	0.43
1:A:866:GLU:HG3	1:A:867:ARG:N	2.33	0.43
1:B:162:MET:HB3	1:B:313:MET:SD	2.58	0.43
1:B:367:ILE:HG22	1:B:489:THR:HG23	1.98	0.43
1:C:222:THR:CG2	1:C:223:PRO:HD3	2.47	0.43
1:C:963:ALA:O	1:C:965:LEU:N	2.51	0.43
1:B:358:PHE:CD1	1:B:977:MET:HB3	2.54	0.43
1:B:848:ALA:C	1:B:850:LYS:H	2.26	0.43
1:B:894:SER:OG	1:B:897:ILE:HG23	2.18	0.43
1:B:952:LEU:C	1:B:954:ASP:H	2.27	0.43
1:C:65:ILE:HD13	1:C:111:LEU:CD2	2.47	0.43
1:C:779:TYR:CD2	1:C:779:TYR:N	2.85	0.43
1:C:901:VAL:O	1:C:904:VAL:CG2	2.60	0.43
1:A:221:GLY:H	1:B:622:GLN:NE2	2.16	0.43
1:A:680:PHE:CD1	1:A:680:PHE:C	2.97	0.43
1:B:25:LEU:HD11	1:C:879:ILE:HG12	1.99	0.43
1:B:129:VAL:HG23	1:C:109:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PRO:HG3	1:C:469:GLN:HG3	2.01	0.43
1:C:418:ARG:NH1	1:C:970:MET:HG2	2.20	0.43
1:C:467:TYR:O	1:C:468:ARG:C	2.61	0.43
1:C:707:ALA:O	1:C:710:PRO:HD3	2.18	0.43
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.83	0.43
1:A:138:MET:HB2	1:A:327:TYR:O	2.19	0.43
1:A:216:ALA:HA	1:B:751:GLY:HA2	2.00	0.43
1:A:547:ILE:HD13	1:A:547:ILE:HA	1.95	0.43
1:B:189:ASN:C	1:B:189:ASN:HD22	2.26	0.43
1:C:393:LEU:CD1	1:C:466:ILE:HG23	2.48	0.43
1:C:456:MET:O	1:C:459:PHE:HD2	2.00	0.43
1:C:591:LEU:HD12	1:C:611:ALA:HB1	2.00	0.43
1:C:609:VAL:HG22	1:C:629:VAL:HG22	2.01	0.43
1:C:687:GLN:HE21	1:C:687:GLN:HB3	1.52	0.43
1:A:431:THR:O	1:A:435:MET:HB2	2.18	0.43
1:A:1024:VAL:O	1:A:1028:VAL:HG23	2.19	0.43
1:B:119:PRO:HG2	1:B:122:VAL:HG21	2.00	0.43
1:B:190:PRO:HD3	1:B:779:TYR:CD2	2.53	0.43
1:B:307:ARG:HH11	1:B:307:ARG:HB2	1.83	0.43
1:C:672:VAL:HG13	1:C:675:GLY:N	2.33	0.43
1:C:742:SER:OG	1:C:745:ASP:HB2	2.18	0.43
1:A:568:ASP:OD2	1:A:637:ARG:NH1	2.52	0.43
1:A:584:GLN:N	1:A:622:GLN:HB3	2.33	0.43
1:A:685:ILE:HB	1:A:687:GLN:HE22	1.83	0.43
1:A:979:SER:O	1:A:983:ILE:HG12	2.17	0.43
1:B:166:ILE:HD11	1:B:310:LEU:CD2	2.48	0.43
1:B:686:ASP:OD2	1:B:686:ASP:C	2.61	0.43
1:B:764:ASP:C	1:B:766:GLY:N	2.76	0.43
1:B:921:LEU:HD21	1:B:1002:ALA:HA	2.00	0.43
1:C:115:MET:HA	1:C:118:LEU:CD2	2.49	0.43
1:A:66:GLU:C	1:A:68:ASN:N	2.77	0.43
1:A:293:LEU:HB3	1:A:294:ALA:H	1.68	0.43
1:A:449:LEU:O	1:A:453:PHE:CD1	2.70	0.43
1:A:566:ASP:HB3	1:A:667:ASN:HD22	1.82	0.43
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.53	0.43
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.54	0.43
1:B:200:PRO:CD	1:B:749:THR:HG23	2.49	0.43
1:B:463:THR:OG1	1:B:464:GLY:N	2.52	0.43
1:B:564:LEU:HD22	1:B:926:TYR:CE2	2.53	0.43
1:B:674:LEU:O	1:B:676:THR:N	2.51	0.43
1:B:705:GLU:HG3	1:B:847:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HA	1:A:128:SER:O	2.19	0.43
1:B:235:ILE:O	1:C:728:LYS:HD2	2.19	0.43
1:B:338:HIS:CE1	1:B:342:LYS:HE3	2.54	0.43
1:C:470:PHE:O	1:C:471:SER:C	2.62	0.43
1:C:520:PHE:O	1:C:522:LYS:N	2.52	0.43
1:C:741:VAL:HG11	1:C:746:ILE:HD11	2.01	0.43
1:C:888:LEU:HD13	1:C:901:VAL:HG23	2.00	0.43
1:B:32:VAL:O	1:B:33:ALA:HB2	2.18	0.43
1:B:49:TYR:HE1	1:B:60:THR:HG21	1.84	0.43
1:B:327:TYR:HB2	1:B:628:PHE:HB3	2.01	0.43
1:B:404:LEU:HD21	1:B:937:LEU:CD2	2.49	0.43
1:B:470:PHE:O	1:B:473:THR:N	2.52	0.43
1:C:83:ASP:HB2	1:C:87:THR:HB	2.01	0.43
1:C:400:LEU:HD12	1:C:933:THR:HG21	1.99	0.43
1:C:695:LEU:HD22	1:C:825:MET:HE3	2.01	0.43
1:C:940:LYS:HA	1:C:943:ILE:HD12	2.01	0.43
1:A:18:ILE:O	1:A:19:ILE:C	2.61	0.43
1:B:234:ILE:C	1:B:235:ILE:HD13	2.44	0.43
1:B:335:ILE:O	1:B:336:SER:C	2.61	0.43
1:B:852:PRO:O	1:B:853:THR:OG1	2.24	0.43
1:B:947:GLU:HA	1:B:947:GLU:OE2	2.18	0.43
1:B:1013:THR:O	1:B:1017:LEU:HB3	2.18	0.43
1:C:61:VAL:HA	1:C:118:LEU:HD12	2.00	0.43
1:C:658:ILE:O	1:C:659:LYS:HD2	2.18	0.43
1:C:672:VAL:HG12	1:C:672:VAL:O	2.18	0.43
1:C:953:MET:SD	1:C:963:ALA:CB	3.07	0.43
1:C:983:ILE:HD13	1:C:1008:MET:HA	2.00	0.43
1:C:1010:GLY:C	1:C:1013:THR:HG22	2.44	0.43
1:C:1022:VAL:HA	1:C:1025:PHE:CE2	2.54	0.43
1:B:154:ILE:O	1:B:157:TYR:N	2.52	0.42
1:B:192:GLU:O	1:B:196:PHE:CD2	2.71	0.42
1:C:65:ILE:O	1:C:66:GLU:C	2.62	0.42
1:C:192:GLU:HG2	1:C:264:ASP:O	2.19	0.42
1:C:355:MET:SD	1:C:410:ILE:HD11	2.59	0.42
1:C:690:LEU:HD11	1:C:854:GLY:HA3	2.00	0.42
1:C:983:ILE:HG23	1:C:1008:MET:HG3	2.01	0.42
1:A:476:SER:O	1:A:480:LEU:HB2	2.19	0.42
1:A:736:ALA:HA	1:A:741:VAL:HG12	2.02	0.42
1:B:111:LEU:HD21	1:B:127:VAL:CG1	2.50	0.42
1:B:349:ILE:HG22	1:B:350:LEU:HD23	2.01	0.42
1:B:547:ILE:HD13	1:B:547:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:VAL:CG1	1:C:326:PRO:HG2	2.49	0.42
1:C:189:ASN:HD21	1:C:191:ASN:HB2	1.84	0.42
1:C:687:GLN:OE1	1:C:856:GLY:HA3	2.18	0.42
1:C:710:PRO:C	1:C:712:MET:H	2.25	0.42
1:A:69:MET:HG3	1:A:92:LEU:HD21	2.00	0.42
1:A:191:ASN:C	1:A:193:LEU:N	2.76	0.42
1:A:317:PHE:HA	1:A:318:PRO:HD2	1.73	0.42
1:A:324:VAL:C	1:A:325:TYR:CD1	2.98	0.42
1:A:566:ASP:HB3	1:A:667:ASN:ND2	2.34	0.42
1:A:733:GLN:O	1:A:736:ALA:HB3	2.20	0.42
1:B:16:ALA:HB2	1:B:488:LEU:HG	2.01	0.42
1:B:87:THR:HG21	1:B:620:ARG:HH12	1.79	0.42
1:B:140:VAL:HG22	1:B:140:VAL:O	2.18	0.42
1:B:155:SER:OG	1:B:179:GLY:HA3	2.20	0.42
1:B:303:ALA:HA	1:B:306:ILE:HD13	2.00	0.42
1:B:391:ASN:O	1:B:395:MET:HG2	2.20	0.42
1:B:721:LEU:HB3	1:B:814:PRO:HG2	2.01	0.42
1:B:910:ILE:C	1:B:912:ALA:N	2.78	0.42
1:C:395:MET:O	1:C:398:MET:N	2.43	0.42
1:C:597:TYR:CD1	1:C:601:LYS:HG3	2.54	0.42
1:C:952:LEU:HA	1:C:956:GLU:HG2	1.99	0.42
1:A:26:ALA:O	1:A:27:ILE:C	2.63	0.42
1:A:180:SER:O	1:A:181:GLN:CB	2.67	0.42
1:B:24:GLY:CA	1:B:27:ILE:HG23	2.49	0.42
1:B:96:SER:HB3	1:B:461:GLY:HA2	2.00	0.42
1:B:190:PRO:CD	1:B:779:TYR:CE2	3.01	0.42
1:B:216:ALA:O	1:B:234:ILE:HB	2.20	0.42
1:B:327:TYR:HD1	1:B:327:TYR:O	2.03	0.42
1:B:335:ILE:HG13	1:B:634:TRP:HD1	1.82	0.42
1:B:830:GLN:HB2	1:B:831:ALA:H	1.62	0.42
1:B:1012:VAL:CG2	1:B:1013:THR:H	2.32	0.42
1:C:406:VAL:CG1	1:C:407:ASP:N	2.82	0.42
1:C:554:TYR:HD1	1:C:558:ARG:NE	2.17	0.42
1:C:783:PRO:C	1:C:785:ASP:H	2.28	0.42
1:A:104:GLN:O	1:A:105:VAL:C	2.63	0.42
1:A:240:LEU:HD12	1:A:240:LEU:N	2.35	0.42
1:A:358:PHE:HB3	1:A:977:MET:HE3	2.01	0.42
1:A:456:MET:C	1:A:458:PHE:H	2.27	0.42
1:A:959:GLY:O	1:A:961:ILE:N	2.53	0.42
1:A:988:PRO:HB2	1:A:989:LEU:H	1.66	0.42
1:B:190:PRO:HG3	1:B:789:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:LEU:HB2	1:C:260:VAL:O	2.19	0.42
1:C:489:THR:N	1:C:490:PRO:HD2	2.34	0.42
1:C:490:PRO:C	1:C:491:ALA:O	2.60	0.42
1:A:34:GLN:HG2	1:A:35:TYR:CE1	2.55	0.42
1:A:51:GLY:C	1:C:215:ALA:HB1	2.45	0.42
1:A:211:ASN:HA	1:A:240:LEU:HD13	2.02	0.42
1:A:693:GLU:O	1:A:694:LYS:C	2.61	0.42
1:A:993:THR:HB	1:A:994:GLY:H	1.74	0.42
1:B:185:ARG:HA	1:B:185:ARG:HD3	1.82	0.42
1:B:858:ASP:OD1	1:B:859:TRP:N	2.48	0.42
1:C:325:TYR:N	1:C:325:TYR:HD1	2.14	0.42
1:C:343:THR:CG2	1:C:989:LEU:HD13	2.42	0.42
1:C:601:LYS:C	1:C:603:LYS:N	2.74	0.42
1:A:577:GLN:HE21	1:A:577:GLN:HB2	1.62	0.42
1:B:57:VAL:O	1:B:58:GLN:C	2.63	0.42
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.89	0.42
1:B:401:ALA:HA	1:B:404:LEU:HB2	2.02	0.42
1:B:682:PHE:HB2	1:B:859:TRP:CZ3	2.55	0.42
1:B:819:TYR:OH	1:B:860:THR:HB	2.20	0.42
1:B:833:PRO:O	1:B:834:GLY:O	2.37	0.42
1:B:946:VAL:HG21	1:B:1026:PHE:CE2	2.55	0.42
1:C:186:ILE:HG13	1:C:268:ILE:HD13	2.00	0.42
1:C:295:THR:HG23	1:C:295:THR:O	2.20	0.42
1:C:768:VAL:C	1:C:769:LYS:HG2	2.43	0.42
1:A:99:ASP:OD1	1:A:101:ASP:N	2.52	0.42
1:A:713:LEU:CD2	1:A:714:THR:H	2.27	0.42
1:A:830:GLN:HE21	1:A:831:ALA:H	1.68	0.42
1:B:181:GLN:CD	1:B:769:LYS:HD3	2.45	0.42
1:B:210:GLN:HE22	1:B:249:ILE:HA	1.85	0.42
1:B:552:MET:C	1:B:554:TYR:N	2.77	0.42
1:B:699:ARG:CG	1:B:700:ASN:H	2.28	0.42
1:B:911:GLY:HA3	1:B:1013:THR:HG21	2.02	0.42
1:C:445:ILE:O	1:C:448:VAL:N	2.53	0.42
1:C:446:ALA:HB2	1:C:482:VAL:HG21	2.02	0.42
1:C:575:MET:SD	1:C:575:MET:N	2.92	0.42
1:C:905:VAL:CB	1:C:906:PRO:HD3	2.47	0.42
1:C:934:THR:C	1:C:936:GLY:N	2.78	0.42
1:C:942:ALA:HB1	1:C:1022:VAL:HG21	2.01	0.42
1:A:696:THR:OG1	1:A:825:MET:HE1	2.20	0.42
1:A:780:ARG:HH22	1:C:223:PRO:CD	2.32	0.42
1:A:828:LEU:HA	1:A:828:LEU:HD23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PRO:C	1:B:121:GLU:N	2.76	0.42
1:B:293:LEU:CD1	1:B:297:ALA:HB3	2.50	0.42
1:B:700:ASN:O	1:B:704:ALA:CB	2.68	0.42
1:B:941:ASN:ND2	1:B:1014:ALA:O	2.50	0.42
1:C:425:LEU:H	1:C:426:PRO:CD	2.33	0.42
1:C:538:THR:HG22	1:C:539:GLY:N	2.30	0.42
1:A:52:ALA:HB3	1:A:86:GLY:CA	2.44	0.42
1:A:341:VAL:O	1:A:345:VAL:HG23	2.20	0.42
1:A:552:MET:HB3	1:A:910:ILE:HG23	2.01	0.42
1:B:137:LEU:HD13	1:B:293:LEU:HG	2.02	0.42
1:B:409:ALA:HB2	1:B:485:ALA:HB2	2.01	0.42
1:B:556:PHE:HB2	1:B:913:LEU:HD21	2.01	0.42
1:B:686:ASP:HB3	1:B:823:PRO:HG2	2.01	0.42
1:B:708:LYS:C	1:B:710:PRO:HD3	2.45	0.42
1:B:762:PHE:CD2	1:B:771:VAL:HG22	2.55	0.42
1:B:911:GLY:O	1:B:1009:GLY:C	2.63	0.42
1:A:822:LEU:HD12	1:A:822:LEU:HA	1.81	0.41
1:A:882:ILE:O	1:A:886:LEU:HB2	2.19	0.41
1:B:11:PHE:CD1	1:C:890:ALA:HB1	2.55	0.41
1:B:166:ILE:O	1:B:168:ARG:N	2.53	0.41
1:B:217:GLY:HA3	1:C:754:TRP:C	2.45	0.41
1:B:251:LEU:HD12	1:B:251:LEU:HA	1.82	0.41
1:B:799:VAL:CG2	1:B:804:PHE:CE2	3.03	0.41
1:B:866:GLU:O	1:B:869:SER:HB3	2.20	0.41
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.48	0.41
1:C:210:GLN:NE2	1:C:249:ILE:HG23	2.35	0.41
1:C:451:ALA:HB1	1:C:883:VAL:HG12	2.02	0.41
1:A:190:PRO:HB3	1:A:789:TRP:CE2	2.55	0.41
1:A:282:ASN:ND2	1:A:609:VAL:H	2.18	0.41
1:A:367:ILE:CG2	1:A:496:MET:HE1	2.40	0.41
1:A:454:VAL:O	1:A:456:MET:O	2.38	0.41
1:A:582:ALA:HB3	1:A:623:ASN:HB2	2.02	0.41
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.55	0.41
1:A:686:ASP:OD2	1:A:690:LEU:HB2	2.20	0.41
1:B:68:ASN:ND2	1:B:114:ALA:HB2	2.34	0.41
1:B:306:ILE:O	1:B:310:LEU:HG	2.20	0.41
1:B:552:MET:SD	1:B:909:VAL:CG2	3.08	0.41
1:B:568:ASP:OD2	1:B:634:TRP:CH2	2.72	0.41
1:C:100:ALA:HB1	1:C:295:THR:HG21	2.01	0.41
1:C:220:GLY:CA	1:C:231:ASN:HD22	2.32	0.41
1:C:577:GLN:O	1:C:577:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:930:GLY:HA3	1:C:1007:VAL:CG2	2.50	0.41
1:A:478:MET:O	1:A:481:SER:HB3	2.19	0.41
1:A:527:TYR:OH	1:A:968:VAL:CG1	2.68	0.41
1:A:754:TRP:HZ2	1:A:786:ILE:HA	1.85	0.41
1:B:282:ASN:C	1:B:284:GLN:N	2.78	0.41
1:B:743:ILE:N	1:B:743:ILE:CD1	2.69	0.41
1:C:393:LEU:HD11	1:C:466:ILE:HG23	2.02	0.41
1:C:896:SER:OG	1:C:1033:PHE:HD1	2.03	0.41
1:C:904:VAL:O	1:C:906:PRO:N	2.54	0.41
1:A:368:PRO:HB3	1:A:409:ALA:HB1	2.02	0.41
1:A:574:THR:HG21	1:A:594:VAL:HG11	2.01	0.41
1:A:598:TYR:O	1:A:602:GLU:HB2	2.20	0.41
1:A:994:GLY:H	1:A:997:SER:HB3	1.85	0.41
1:B:314:GLU:H	1:B:315:PRO:HD3	1.86	0.41
1:B:493:CYS:O	1:B:497:LEU:HB3	2.18	0.41
1:B:600:THR:O	1:B:602:GLU:N	2.50	0.41
1:B:650:ARG:O	1:B:654:ALA:N	2.44	0.41
1:B:46:SER:HA	1:B:88:VAL:O	2.21	0.41
1:B:150:THR:O	1:B:151:GLN:C	2.64	0.41
1:B:230:LEU:HD13	1:B:230:LEU:C	2.45	0.41
1:B:445:ILE:HG13	1:B:940:LYS:CG	2.50	0.41
1:C:189:ASN:HD22	1:C:190:PRO:N	2.18	0.41
1:A:111:LEU:O	1:A:113:LEU:N	2.53	0.41
1:A:551:GLY:O	1:A:555:LEU:HD23	2.21	0.41
1:B:20:MET:CG	1:B:374:VAL:HA	2.51	0.41
1:B:72:ILE:HD11	1:B:75:LEU:HD22	2.01	0.41
1:B:485:ALA:HA	1:B:489:THR:HB	2.02	0.41
1:C:425:LEU:H	1:C:426:PRO:HD3	1.85	0.41
1:C:688:ALA:O	1:C:689:GLY:C	2.62	0.41
1:A:534:ILE:HB	1:A:541:TYR:CE2	2.56	0.41
1:A:568:ASP:OD1	1:A:634:TRP:CZ3	2.74	0.41
1:A:617:PHE:CE1	1:A:626:ILE:HD11	2.55	0.41
1:A:681:ASP:H	1:A:863:SER:HB3	1.86	0.41
1:B:254:ASN:HD22	1:B:254:ASN:HA	1.58	0.41
1:B:699:ARG:C	1:B:701:GLN:N	2.78	0.41
1:C:13:TRP:O	1:C:17:ILE:HG13	2.20	0.41
1:C:119:PRO:HG2	1:C:122:VAL:CG2	2.51	0.41
1:C:350:LEU:HD21	1:C:984:LEU:HD22	2.03	0.41
1:C:736:ALA:C	1:C:738:ALA:N	2.78	0.41
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.82	0.41
1:A:355:MET:HE1	1:A:413:VAL:CG1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ALA:HB1	1:A:716:VAL:HG11	2.02	0.41
1:B:535:LEU:HD11	1:B:1023:PRO:O	2.20	0.41
1:B:704:ALA:O	1:B:705:GLU:CB	2.64	0.41
1:C:735:LYS:O	1:C:739:LEU:HD13	2.20	0.41
1:C:982:PHE:O	1:C:983:ILE:C	2.64	0.41
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.56	0.41
1:A:150:THR:HG1	1:A:153:ASP:CG	2.29	0.41
1:A:516:PHE:CE2	1:A:520:PHE:HB2	2.56	0.41
1:A:724:THR:HG22	1:A:725:PRO:O	2.21	0.41
1:B:157:TYR:HA	1:B:161:ASN:HD22	1.86	0.41
1:B:181:GLN:HE21	1:B:181:GLN:HB3	1.52	0.41
1:B:280:GLU:CB	1:B:284:GLN:O	2.63	0.41
1:B:369:THR:O	1:B:372:VAL:HG13	2.21	0.41
1:B:439:GLN:HA	1:B:442:LEU:HD12	2.03	0.41
1:B:541:TYR:O	1:B:543:VAL:N	2.54	0.41
1:B:578:LEU:HD23	1:B:578:LEU:N	2.36	0.41
1:B:1004:GLY:O	1:B:1006:GLY:N	2.54	0.41
1:B:1012:VAL:HG23	1:B:1013:THR:H	1.83	0.41
1:C:158:VAL:HG11	1:C:177:LEU:CD2	2.49	0.41
1:C:189:ASN:ND2	1:C:191:ASN:N	2.66	0.41
1:C:575:MET:HE2	3:C:2002:RFP:O12	2.20	0.41
1:C:648:THR:OG1	1:C:649:MET:N	2.53	0.41
1:C:655:PHE:C	1:C:657:GLN:H	2.28	0.41
1:C:712:MET:SD	1:C:843:LEU:HD22	2.61	0.41
1:C:733:GLN:CD	1:C:743:ILE:HG12	2.46	0.41
1:C:836:SER:HB3	1:C:839:GLU:HG3	2.03	0.41
1:C:919:ARG:HB3	1:C:921:LEU:HD23	2.03	0.41
1:C:987:MET:SD	1:C:1008:MET:HE1	2.61	0.41
1:C:997:SER:OG	1:C:998:GLY:N	2.54	0.41
1:A:38:ILE:HD13	1:A:38:ILE:H	1.86	0.41
1:A:712:MET:HE1	1:A:839:GLU:HG3	2.02	0.41
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.48	0.41
1:A:886:LEU:HD12	1:A:886:LEU:HA	1.94	0.41
1:A:1029:VAL:O	1:A:1030:ARG:CB	2.66	0.41
1:B:370:ILE:HD13	1:B:370:ILE:HA	1.93	0.41
1:B:415:ASN:HD21	1:B:971:ARG:HG2	1.86	0.41
1:B:1033:PHE:O	1:B:1034:SER:CB	2.68	0.41
1:C:467:TYR:C	1:C:469:GLN:N	2.77	0.41
1:A:20:MET:HG2	1:A:377:LEU:HD22	2.01	0.40
1:A:113:LEU:HD23	1:C:127:VAL:O	2.21	0.40
1:A:213:GLN:HE21	1:A:213:GLN:HB2	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ILE:O	1:A:787:GLY:C	2.64	0.40
1:A:904:VAL:O	1:A:905:VAL:C	2.63	0.40
1:B:40:PRO:HB2	1:B:94:PHE:O	2.21	0.40
1:B:114:ALA:O	1:B:115:MET:C	2.64	0.40
1:B:265:VAL:HG22	1:B:265:VAL:O	2.20	0.40
1:B:761:ASP:HB3	1:B:768:VAL:HG13	2.04	0.40
1:B:986:VAL:HG12	1:B:990:VAL:HG22	2.01	0.40
1:C:223:PRO:HA	1:C:224:PRO:HD3	1.92	0.40
1:C:323:ILE:HG22	1:C:325:TYR:CE1	2.56	0.40
1:C:552:MET:HE3	1:C:552:MET:HB2	1.84	0.40
1:C:930:GLY:HA3	1:C:1007:VAL:HG22	2.03	0.40
1:C:1020:PHE:C	1:C:1023:PRO:HD2	2.47	0.40
1:A:574:THR:OG1	1:A:598:TYR:HE1	2.04	0.40
1:A:708:LYS:C	1:A:710:PRO:HD3	2.47	0.40
1:A:742:SER:O	1:A:744:ASN:N	2.55	0.40
1:A:758:TYR:CE1	1:A:770:LYS:HB3	2.56	0.40
1:A:911:GLY:CA	1:A:914:LEU:HB2	2.49	0.40
1:B:115:MET:SD	1:B:127:VAL:HG11	2.61	0.40
1:B:909:VAL:O	1:B:913:LEU:HD22	2.21	0.40
1:C:795:ASP:OD2	1:C:795:ASP:C	2.64	0.40
1:C:815:ARG:CZ	3:C:2002:RFP:H302	2.50	0.40
1:C:965:LEU:HB3	1:C:966:ASP:H	1.61	0.40
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.57	0.40
1:A:333:VAL:O	1:A:337:ILE:HB	2.22	0.40
1:A:438:ILE:O	1:A:439:GLN:C	2.64	0.40
1:A:578:LEU:CD2	1:A:587:THR:HG23	2.52	0.40
1:A:872:GLN:O	1:A:873:ALA:C	2.63	0.40
1:A:961:ILE:HD12	1:A:1031:ARG:HH22	1.86	0.40
1:B:36:PRO:HG3	1:B:469:GLN:CD	2.45	0.40
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.56	0.40
1:B:327:TYR:CD2	1:B:628:PHE:HB3	2.57	0.40
1:C:210:GLN:HE22	1:C:250:LEU:H	1.69	0.40
1:C:631:LEU:HB2	1:C:637:ARG:NH2	2.36	0.40
1:C:1015:THR:O	1:C:1019:ILE:HB	2.22	0.40
1:A:126:GLY:CA	1:B:116:PRO:HB3	2.43	0.40
1:A:591:LEU:HD23	1:A:591:LEU:HA	1.96	0.40
1:B:5:PHE:HB3	1:B:12:ALA:HB2	2.03	0.40
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.83	0.40
1:B:289:LEU:CD1	1:B:289:LEU:N	2.84	0.40
1:B:613:ASN:O	1:B:615:PHE:N	2.49	0.40
1:B:754:TRP:CH2	1:B:785:ASP:HB2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:TYR:CD1	1:B:864:TYR:C	2.99	0.40
1:C:686:ASP:OD2	1:C:690:LEU:N	2.54	0.40
1:C:717:ARG:NH2	3:C:2002:RFP:O8	2.53	0.40
3:C:2002:RFP:H311	3:C:2002:RFP:H323	2.03	0.40
1:A:12:ALA:O	1:A:488:LEU:HD13	2.21	0.40
1:A:883:VAL:O	1:A:883:VAL:HG12	2.20	0.40
1:B:4:PHE:O	1:B:5:PHE:CB	2.69	0.40
1:B:95:GLU:O	1:B:96:SER:C	2.62	0.40
1:B:262:LEU:HA	1:B:265:VAL:HG12	2.04	0.40
1:C:34:GLN:HB2	1:C:35:TYR:CZ	2.56	0.40
1:C:762:PHE:CE2	1:C:764:ASP:HB2	2.56	0.40
1:C:832:ALA:CB	1:C:833:PRO:CD	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1018/1053 (97%)	752 (74%)	173 (17%)	93 (9%)	0	3
1	B	1018/1053 (97%)	730 (72%)	201 (20%)	87 (8%)	0	4
1	C	1018/1053 (97%)	760 (75%)	178 (18%)	80 (8%)	1	5
All	All	3054/3159 (97%)	2242 (73%)	552 (18%)	260 (8%)	0	4

All (260) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	181	GLN
1	A	182	TYR
1	A	282	ASN
1	A	293	LEU

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Mol	Chain	Res	Type
1	A	294	ALA
1	A	319	SER
1	A	388	PHE
1	A	392	THR
1	A	439	GLN
1	A	580	ALA
1	A	601	LYS
1	A	659	LYS
1	A	661	ALA
1	A	677	ALA
1	A	678	THR
1	A	713	LEU
1	A	715	SER
1	A	746	ILE
1	A	831	ALA
1	A	893	GLU
1	A	960	LEU
1	A	992	SER
1	A	1016	VAL
1	B	2	PRO
1	B	22	ALA
1	B	54	ALA
1	B	124	GLN
1	B	147	GLY
1	B	228	GLN
1	B	262	LEU
1	B	326	PRO
1	B	358	PHE
1	B	583	THR
1	B	601	LYS
1	B	633	ASP
1	B	638	PRO
1	B	640	GLU
1	B	656	SER
1	B	669	PRO
1	B	671	ILE
1	B	675	GLY
1	B	676	THR
1	B	733	GLN
1	B	775	SER
1	B	806	SER
1	B	918	PHE

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Mol	Chain	Res	Type
1	B	1016	VAL
1	B	1021	PHE
1	B	1034	SER
1	C	226	LYS
1	C	266	ALA
1	C	326	PRO
1	C	463	THR
1	C	464	GLY
1	C	520	PHE
1	C	553	ALA
1	C	580	ALA
1	C	602	GLU
1	C	678	THR
1	C	720	GLY
1	C	806	SER
1	C	832	ALA
1	C	869	SER
1	C	872	GLN
1	C	905	VAL
1	C	921	LEU
1	C	960	LEU
1	C	965	LEU
1	C	993	THR
1	C	998	GLY
1	A	19	ILE
1	A	52	ALA
1	A	64	VAL
1	A	95	GLU
1	A	134	SER
1	A	170	SER
1	A	221	GLY
1	A	256	ASP
1	A	354	VAL
1	A	358	PHE
1	A	362	PHE
1	A	424	GLY
1	A	428	LYS
1	A	460	GLY
1	A	534	ILE
1	A	638	PRO
1	A	675	GLY
1	A	743	ILE

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Mol	Chain	Res	Type
1	A	870	GLY
1	A	903	LEU
1	A	958	LYS
1	A	975	ILE
1	A	988	PRO
1	A	998	GLY
1	A	1017	LEU
1	A	1034	SER
1	B	140	VAL
1	B	216	ALA
1	B	227	GLY
1	B	243	THR
1	B	361	ASN
1	B	486	LEU
1	B	542	LEU
1	B	580	ALA
1	B	613	ASN
1	B	654	ALA
1	B	666	PHE
1	B	672	VAL
1	B	690	LEU
1	B	705	GLU
1	B	834	GLY
1	B	852	PRO
1	B	899	PHE
1	B	953	MET
1	B	1005	THR
1	C	86	GLY
1	C	255	GLN
1	C	438	ILE
1	C	521	GLU
1	C	601	LYS
1	C	656	SER
1	C	674	LEU
1	C	711	ASP
1	C	713	LEU
1	C	952	LEU
1	C	953	MET
1	C	997	SER
1	C	1027	VAL
1	A	53	ASP
1	A	112	GLN

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Mol	Chain	Res	Type
1	A	167	SER
1	A	174	ASP
1	A	236	ALA
1	A	436	GLY
1	A	452	VAL
1	A	618	ALA
1	B	167	SER
1	B	222	THR
1	B	319	SER
1	B	360	GLN
1	B	439	GLN
1	B	517	ASN
1	B	540	ARG
1	B	553	ALA
1	B	585	GLU
1	B	618	ALA
1	B	655	PHE
1	B	677	ALA
1	B	723	ASP
1	B	765	ARG
1	B	794	ALA
1	B	889	ALA
1	B	968	VAL
1	C	285	PRO
1	C	328	ASP
1	C	336	SER
1	C	427	PRO
1	C	468	ARG
1	C	554	TYR
1	C	555	LEU
1	C	620	ARG
1	C	636	ASP
1	C	658	ILE
1	C	712	MET
1	C	721	LEU
1	C	722	GLU
1	C	756	GLY
1	C	873	ALA
1	C	994	GLY
1	A	317	PHE
1	A	376	LEU
1	A	427	PRO

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Mol	Chain	Res	Type
1	A	517	ASN
1	A	539	GLY
1	A	953	MET
1	A	987	MET
1	B	120	GLN
1	B	127	VAL
1	B	453	PHE
1	B	796	GLY
1	B	820	ASN
1	B	909	VAL
1	C	377	LEU
1	C	425	LEU
1	C	497	LEU
1	C	541	TYR
1	C	675	GLY
1	C	802	SER
1	C	885	PHE
1	C	974	PRO
1	C	983	ILE
1	A	133	SER
1	A	180	SER
1	A	334	LYS
1	A	347	ALA
1	A	421	ALA
1	A	456	MET
1	A	689	GLY
1	A	1030	ARG
1	B	440	GLY
1	B	442	LEU
1	B	515	TRP
1	B	614	GLY
1	B	851	LEU
1	B	974	PRO
1	B	1017	LEU
1	C	62	THR
1	C	477	ALA
1	C	552	MET
1	C	825	MET
1	C	964	THR
1	C	967	ALA
1	A	9	PRO
1	A	18	ILE

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Mol	Chain	Res	Type
1	A	220	GLY
1	A	268	ILE
1	A	318	PRO
1	A	330	THR
1	A	360	GLN
1	A	496	MET
1	A	687	GLN
1	B	125	GLN
1	B	283	GLY
1	B	602	GLU
1	B	921	LEU
1	C	332	PHE
1	C	343	THR
1	C	751	GLY
1	C	784	ASP
1	C	1005	THR
1	C	1035	ARG
1	A	105	VAL
1	A	351	VAL
1	B	86	GLY
1	C	1028	VAL
1	A	38	ILE
1	A	335	ILE
1	B	975	ILE
1	C	935	ILE
1	C	1006	GLY
1	A	15	ILE
1	A	139	VAL
1	A	320	GLY
1	A	410	ILE
1	A	787	GLY
1	B	201	VAL
1	B	306	ILE
1	C	15	ILE
1	A	461	GLY
1	B	223	PRO
1	B	647	ILE
1	B	874	PRO
1	B	961	ILE
1	C	222	THR
1	C	224	PRO
1	C	671	ILE

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Mol	Chain	Res	Type
1	C	975	ILE
1	C	1016	VAL
1	A	340	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	833/859 (97%)	692 (83%)	141 (17%)	2	10
1	B	833/859 (97%)	690 (83%)	143 (17%)	2	10
1	C	833/859 (97%)	690 (83%)	143 (17%)	2	10
All	All	2499/2577 (97%)	2072 (83%)	427 (17%)	2	10

All (427) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	25	LEU
1	A	38	ILE
1	A	44	THR
1	A	57	VAL
1	A	58	GLN
1	A	60	THR
1	A	63	GLN
1	A	65	ILE
1	A	69	MET
1	A	70	ASN
1	A	72	ILE
1	A	76	MET
1	A	88	VAL
1	A	96	SER
1	A	105	VAL
1	A	109	ASN
1	A	110	LYS
1	A	111	LEU

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Mol	Chain	Res	Type
1	A	117	LEU
1	A	120	GLN
1	A	131	LYS
1	A	143	ILE
1	A	164	ASP
1	A	176	GLN
1	A	181	GLN
1	A	193	LEU
1	A	207	ILE
1	A	210	GLN
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	234	ILE
1	A	243	THR
1	A	250	LEU
1	A	255	GLN
1	A	260	VAL
1	A	277	ILE
1	A	284	GLN
1	A	289	LEU
1	A	293	LEU
1	A	298	ASN
1	A	302	THR
1	A	323	ILE
1	A	337	ILE
1	A	341	VAL
1	A	358	PHE
1	A	359	LEU
1	A	360	GLN
1	A	361	ASN
1	A	367	ILE
1	A	372	VAL
1	A	376	LEU
1	A	377	LEU
1	A	379	THR
1	A	382	VAL
1	A	394	THR
1	A	405	LEU
1	A	406	VAL
1	A	410	ILE
1	A	414	GLU

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Mol	Chain	Res	Type
1	A	417	GLU
1	A	418	ARG
1	A	422	GLU
1	A	423	GLU
1	A	448	VAL
1	A	454	VAL
1	A	462	SER
1	A	473	THR
1	A	475	VAL
1	A	476	SER
1	A	480	LEU
1	A	483	LEU
1	A	489	THR
1	A	496	MET
1	A	516	PHE
1	A	530	SER
1	A	534	ILE
1	A	537	SER
1	A	540	ARG
1	A	542	LEU
1	A	544	LEU
1	A	547	ILE
1	A	549	VAL
1	A	550	VAL
1	A	563	PHE
1	A	576	VAL
1	A	577	GLN
1	A	578	LEU
1	A	583	THR
1	A	586	ARG
1	A	589	LYS
1	A	597	TYR
1	A	624	THR
1	A	626	ILE
1	A	630	SER
1	A	645	GLU
1	A	649	MET
1	A	658	ILE
1	A	659	LYS
1	A	668	LEU
1	A	671	ILE
1	A	680	PHE

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Mol	Chain	Res	Type
1	A	684	LEU
1	A	686	ASP
1	A	687	GLN
1	A	713	LEU
1	A	714	THR
1	A	741	VAL
1	A	750	LEU
1	A	768	VAL
1	A	773	VAL
1	A	780	ARG
1	A	808	ARG
1	A	810	GLU
1	A	815	ARG
1	A	817	GLU
1	A	822	LEU
1	A	843	LEU
1	A	865	GLN
1	A	866	GLU
1	A	867	ARG
1	A	881	LEU
1	A	887	CYS
1	A	904	VAL
1	A	933	THR
1	A	935	ILE
1	A	952	LEU
1	A	960	LEU
1	A	961	ILE
1	A	972	LEU
1	A	982	PHE
1	A	989	LEU
1	A	991	ILE
1	A	993	THR
1	A	1001	ASN
1	A	1008	MET
1	A	1011	MET
1	A	1012	VAL
1	A	1017	LEU
1	A	1034	SER
1	B	3	ASN
1	B	8	ARG
1	B	13	TRP
1	B	27	ILE

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Mol	Chain	Res	Type
1	B	30	LEU
1	B	56	THR
1	B	60	THR
1	B	62	THR
1	B	67	GLN
1	B	70	ASN
1	B	72	ILE
1	B	85	THR
1	B	88	VAL
1	B	95	GLU
1	B	104	GLN
1	B	106	GLN
1	B	120	GLN
1	B	121	GLU
1	B	124	GLN
1	B	129	VAL
1	B	137	LEU
1	B	140	VAL
1	B	145	THR
1	B	149	MET
1	B	150	THR
1	B	153	ASP
1	B	155	SER
1	B	156	ASP
1	B	169	THR
1	B	170	SER
1	B	176	GLN
1	B	181	GLN
1	B	189	ASN
1	B	194	ASN
1	B	199	THR
1	B	225	VAL
1	B	230	LEU
1	B	238	THR
1	B	239	ARG
1	B	243	THR
1	B	244	GLU
1	B	253	VAL
1	B	254	ASN
1	B	261	LEU
1	B	280	GLU
1	B	289	LEU

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Mol	Chain	Res	Type
1	B	291	ILE
1	B	292	LYS
1	B	293	LEU
1	B	314	GLU
1	B	324	VAL
1	B	327	TYR
1	B	330	THR
1	B	337	ILE
1	B	343	THR
1	B	359	LEU
1	B	370	ILE
1	B	372	VAL
1	B	399	VAL
1	B	402	ILE
1	B	406	VAL
1	B	408	ASP
1	B	410	ILE
1	B	411	VAL
1	B	414	GLU
1	B	415	ASN
1	B	420	MET
1	B	438	ILE
1	B	445	ILE
1	B	448	VAL
1	B	449	LEU
1	B	452	VAL
1	B	459	PHE
1	B	473	THR
1	B	480	LEU
1	B	488	LEU
1	B	497	LEU
1	B	515	TRP
1	B	534	ILE
1	B	540	ARG
1	B	547	ILE
1	B	557	VAL
1	B	559	LEU
1	B	571	VAL
1	B	578	LEU
1	B	589	LYS
1	B	591	LEU
1	B	601	LYS

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Mol	Chain	Res	Type
1	B	606	VAL
1	B	620	ARG
1	B	622	GLN
1	B	629	VAL
1	B	649	MET
1	B	653	ARG
1	B	655	PHE
1	B	668	LEU
1	B	674	LEU
1	B	690	LEU
1	B	693	GLU
1	B	696	THR
1	B	699	ARG
1	B	702	LEU
1	B	712	MET
1	B	741	VAL
1	B	743	ILE
1	B	750	LEU
1	B	770	LYS
1	B	773	VAL
1	B	774	MET
1	B	779	TYR
1	B	782	LEU
1	B	788	ASP
1	B	795	ASP
1	B	799	VAL
1	B	813	SER
1	B	842	GLU
1	B	846	GLN
1	B	847	LEU
1	B	851	LEU
1	B	868	LEU
1	B	879	ILE
1	B	891	LEU
1	B	900	SER
1	B	913	LEU
1	B	925	VAL
1	B	935	ILE
1	B	952	LEU
1	B	954	ASP
1	B	956	GLU
1	B	958	LYS

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Mol	Chain	Res	Type
1	B	960	LEU
1	B	966	ASP
1	B	978	THR
1	B	984	LEU
1	B	989	LEU
1	B	990	VAL
1	B	991	ILE
1	B	1007	VAL
1	B	1020	PHE
1	B	1022	VAL
1	B	1027	VAL
1	B	1034	SER
1	B	1036	LYS
1	C	8	ARG
1	C	13	TRP
1	C	32	VAL
1	C	35	TYR
1	C	38	ILE
1	C	43	VAL
1	C	44	THR
1	C	46	SER
1	C	56	THR
1	C	63	GLN
1	C	89	GLN
1	C	91	THR
1	C	96	SER
1	C	107	VAL
1	C	111	LEU
1	C	112	GLN
1	C	124	GLN
1	C	125	GLN
1	C	127	VAL
1	C	133	SER
1	C	134	SER
1	C	150	THR
1	C	158	VAL
1	C	166	ILE
1	C	177	LEU
1	C	186	ILE
1	C	189	ASN
1	C	193	LEU
1	C	225	VAL

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Mol	Chain	Res	Type
1	C	226	LYS
1	C	230	LEU
1	C	233	SER
1	C	239	ARG
1	C	240	LEU
1	C	244	GLU
1	C	253	VAL
1	C	259	ARG
1	C	274	ASN
1	C	300	LEU
1	C	306	ILE
1	C	324	VAL
1	C	325	TYR
1	C	341	VAL
1	C	344	LEU
1	C	348	ILE
1	C	349	ILE
1	C	350	LEU
1	C	351	VAL
1	C	355	MET
1	C	356	TYR
1	C	367	ILE
1	C	370	ILE
1	C	372	VAL
1	C	379	THR
1	C	394	THR
1	C	400	LEU
1	C	402	ILE
1	C	408	ASP
1	C	410	ILE
1	C	416	VAL
1	C	417	GLU
1	C	418	ARG
1	C	419	VAL
1	C	429	GLU
1	C	432	ARG
1	C	454	VAL
1	C	472	ILE
1	C	480	LEU
1	C	483	LEU
1	C	492	LEU
1	C	497	LEU

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Mol	Chain	Res	Type
1	C	521	GLU
1	C	522	LYS
1	C	525	HIS
1	C	529	ASP
1	C	542	LEU
1	C	544	LEU
1	C	571	VAL
1	C	577	GLN
1	C	578	LEU
1	C	588	GLN
1	C	591	LEU
1	C	596	HIS
1	C	607	GLU
1	C	609	VAL
1	C	624	THR
1	C	631	LEU
1	C	636	ASP
1	C	644	VAL
1	C	659	LYS
1	C	671	ILE
1	C	673	GLU
1	C	674	LEU
1	C	681	ASP
1	C	684	LEU
1	C	685	ILE
1	C	686	ASP
1	C	687	GLN
1	C	693	GLU
1	C	695	LEU
1	C	697	GLN
1	C	699	ARG
1	C	713	LEU
1	C	714	THR
1	C	715	SER
1	C	722	GLU
1	C	724	THR
1	C	731	ILE
1	C	745	ASP
1	C	750	LEU
1	C	759	VAL
1	C	760	ASN
1	C	765	ARG

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Mol	Chain	Res	Type
1	C	771	VAL
1	C	779	TYR
1	C	791	VAL
1	C	799	VAL
1	C	808	ARG
1	C	847	LEU
1	C	849	SER
1	C	851	LEU
1	C	868	LEU
1	C	869	SER
1	C	871	ASN
1	C	876	LEU
1	C	879	ILE
1	C	900	SER
1	C	901	VAL
1	C	907	LEU
1	C	922	THR
1	C	931	LEU
1	C	934	THR
1	C	941	ASN
1	C	952	LEU
1	C	954	ASP
1	C	964	THR
1	C	982	PHE
1	C	983	ILE
1	C	993	THR
1	C	1017	LEU
1	C	1028	VAL
1	C	1029	VAL
1	C	1035	ARG

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

Mol	Chain	Res	Type
1	A	3	ASN
1	A	58	GLN
1	A	67	GLN
1	A	68	ASN
1	A	70	ASN
1	A	89	GLN
1	A	104	GLN
1	A	106	GLN

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Mol	Chain	Res	Type
1	A	109	ASN
1	A	120	GLN
1	A	124	GLN
1	A	181	GLN
1	A	191	ASN
1	A	210	GLN
1	A	213	GLN
1	A	254	ASN
1	A	282	ASN
1	A	298	ASN
1	A	360	GLN
1	A	361	ASN
1	A	577	GLN
1	A	584	GLN
1	A	588	GLN
1	A	596	HIS
1	A	687	GLN
1	A	719	ASN
1	A	830	GLN
1	A	846	GLN
1	A	865	GLN
1	A	923	ASN
1	A	928	GLN
1	B	34	GLN
1	B	67	GLN
1	B	68	ASN
1	B	70	ASN
1	B	74	ASN
1	B	89	GLN
1	B	104	GLN
1	B	106	GLN
1	B	112	GLN
1	B	125	GLN
1	B	161	ASN
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	274	ASN
1	B	338	HIS

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Mol	Chain	Res	Type
1	B	415	ASN
1	B	517	ASN
1	B	526	HIS
1	B	569	GLN
1	B	605	ASN
1	B	642	ASN
1	B	692	HIS
1	B	701	GLN
1	B	744	ASN
1	B	846	GLN
1	B	865	GLN
1	C	63	GLN
1	C	68	ASN
1	C	89	GLN
1	C	104	GLN
1	C	109	ASN
1	C	123	GLN
1	C	124	GLN
1	C	125	GLN
1	C	144	ASN
1	C	176	GLN
1	C	189	ASN
1	C	194	ASN
1	C	197	GLN
1	C	210	GLN
1	C	211	ASN
1	C	231	ASN
1	C	237	GLN
1	C	274	ASN
1	C	577	GLN
1	C	657	GLN
1	C	667	ASN
1	C	726	GLN
1	C	760	ASN
1	C	830	GLN
1	C	871	ASN
1	C	872	GLN
1	C	923	ASN
1	C	928	GLN
1	C	941	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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$
3	RFP	C	2002	-	63,63,63	2.09	3 (4%)	94,94,94	1.79	14 (14%)
2	MIY	A	2001	-	36,36,36	1.90	3 (8%)	42,58,58	1.81	10 (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
3	RFP	C	2002	-	-	18/60/85/85	0/5/5/5
2	MIY	A	2001	-	-	7/12/70/70	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2002	RFP	O4-C11	14.38	1.43	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	MIY	O5-C15	9.95	1.44	1.23
3	C	2002	RFP	O7-C35	5.66	1.47	1.35
3	C	2002	RFP	O5-C29	3.40	1.48	1.39
2	A	2001	MIY	C18-C1	-2.43	1.51	1.55
2	A	2001	MIY	C16-C15	2.35	1.52	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2002	RFP	O4-C11-C5	-8.82	115.37	131.63
2	A	2001	MIY	O5-C15-C14	-6.12	110.99	122.06
2	A	2001	MIY	O5-C15-C16	-4.89	112.64	121.14
3	C	2002	RFP	O7-C35-C36	4.77	119.60	111.09
3	C	2002	RFP	O4-C11-C12	-4.35	111.82	120.56
3	C	2002	RFP	C41-C42-N4	4.31	117.78	110.86
3	C	2002	RFP	C42-N4-C39	3.69	115.42	109.54
3	C	2002	RFP	O3-C6-C7	3.60	127.26	121.16
3	C	2002	RFP	C12-O5-C29	3.59	126.67	117.84
3	C	2002	RFP	C30-C16-C17	-3.51	115.14	123.67
3	C	2002	RFP	C3-C43-N2	3.09	126.62	121.58
2	A	2001	MIY	C15-C16-C17	2.93	121.12	118.80
3	C	2002	RFP	C12-C11-C5	-2.87	101.75	107.30
3	C	2002	RFP	C2-C3-C43	-2.70	121.12	123.99
2	A	2001	MIY	O2-C3-C2	-2.64	118.51	122.93
2	A	2001	MIY	C71-N7-CN7	-2.52	108.08	116.18
2	A	2001	MIY	C18-C1-C2	2.38	119.54	115.75
2	A	2001	MIY	O6-C17-C18	2.36	116.79	113.37
2	A	2001	MIY	C11-C10-N7	-2.20	118.62	121.65
3	C	2002	RFP	C39-C40-N3	2.18	114.05	110.51
3	C	2002	RFP	C4-C3-C43	2.17	119.41	116.63
2	A	2001	MIY	C13-C14-C15	-2.06	118.40	121.45
2	A	2001	MIY	C18-C5-C4	2.06	114.45	111.64
3	C	2002	RFP	O7-C25-C24	2.02	112.16	107.52

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	MIY	C1-C2-C21-O8
2	A	2001	MIY	C3-C2-C21-O8
2	A	2001	MIY	C1-C2-C21-N2
2	A	2001	MIY	C3-C2-C21-N2

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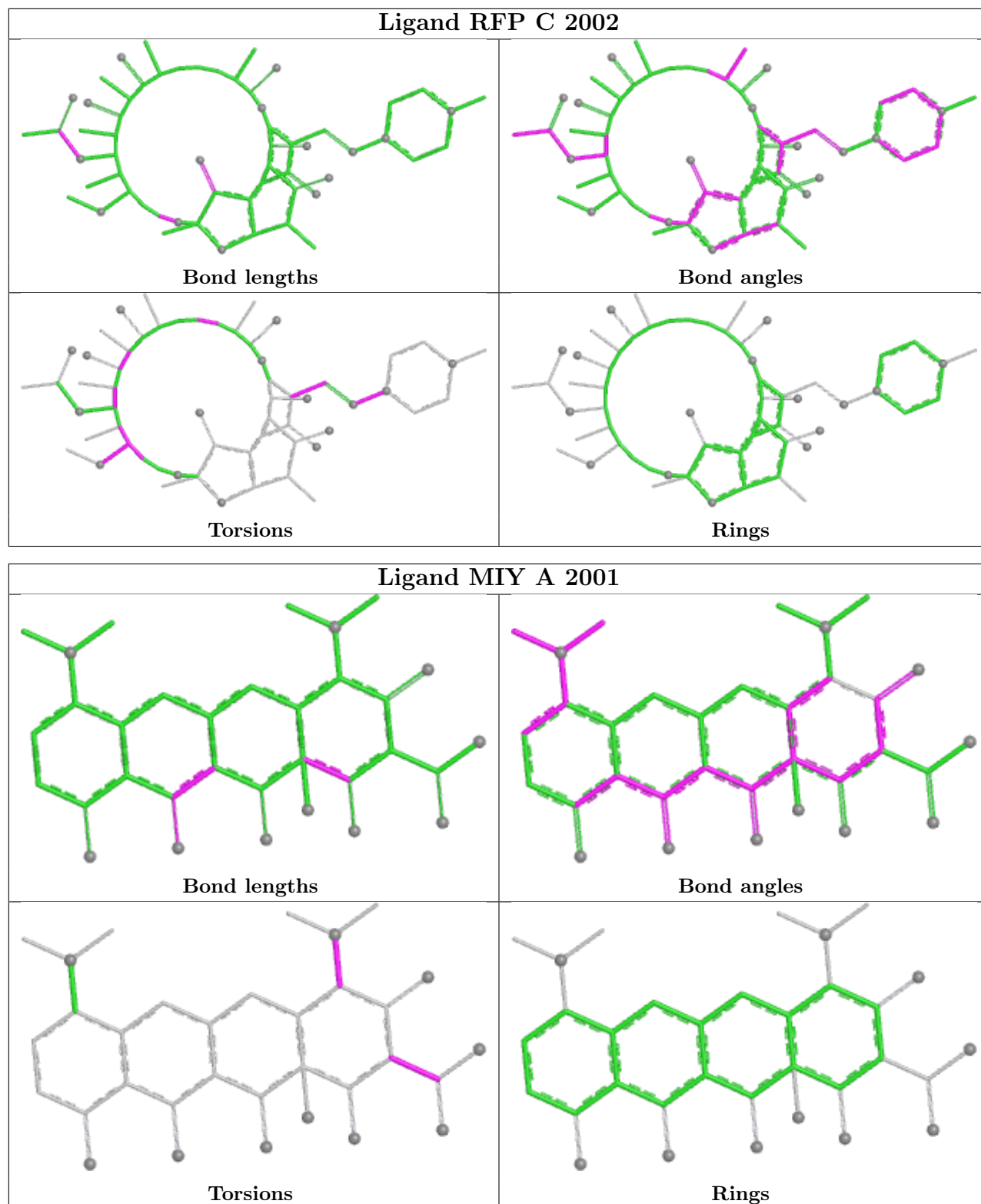
Mol	Chain	Res	Type	Atoms
2	A	2001	MIY	C5-C4-N1-C20
3	C	2002	RFP	C4-C3-C43-N2
3	C	2002	RFP	C26-C27-O6-C37
3	C	2002	RFP	C28-C27-O6-C37
3	C	2002	RFP	C43-N2-N3-C40
3	C	2002	RFP	C43-N2-N3-C41
3	C	2002	RFP	O6-C27-C28-C29
3	C	2002	RFP	C32-C22-C23-C24
3	C	2002	RFP	C21-C22-C23-C24
3	C	2002	RFP	C23-C24-C25-C26
3	C	2002	RFP	C34-C26-C27-C28
3	C	2002	RFP	C25-C26-C27-C28
2	A	2001	MIY	C3-C4-N1-C19
2	A	2001	MIY	C5-C4-N1-C19
3	C	2002	RFP	C33-C24-C25-C26
3	C	2002	RFP	C23-C24-C25-O7
3	C	2002	RFP	C32-C22-C23-O9
3	C	2002	RFP	C16-C17-C18-C19
3	C	2002	RFP	C2-C3-C43-N2
3	C	2002	RFP	C34-C26-C27-O6
3	C	2002	RFP	C25-C26-C27-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2002	RFP	5	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.03	15 (1%)	72 53	52, 102, 136, 167	0
1	B	1022/1053 (97%)	0.11	16 (1%)	70 52	65, 106, 140, 169	0
1	C	1022/1053 (97%)	0.04	15 (1%)	72 53	49, 100, 148, 183	0
All	All	3066/3159 (97%)	0.06	46 (1%)	72 53	49, 103, 142, 183	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	VAL	5.2
1	A	989	LEU	4.0
1	C	514	GLY	3.9
1	C	671	ILE	3.6
1	C	920	GLY	3.4
1	B	960	LEU	3.2
1	B	672	VAL	3.2
1	B	868	LEU	3.1
1	A	960	LEU	3.0
1	A	145	THR	3.0
1	C	960	LEU	2.9
1	C	424	GLY	2.8
1	B	663	VAL	2.8
1	B	968	VAL	2.7
1	A	714	THR	2.5
1	B	1026	PHE	2.5
1	B	535	LEU	2.5
1	B	655	PHE	2.4
1	A	915	ALA	2.4
1	A	957	GLY	2.4
1	B	712	MET	2.4
1	A	871	ASN	2.4
1	A	988	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	917	THR	2.4
1	B	958	LYS	2.4
1	A	972	LEU	2.4
1	B	703	LEU	2.3
1	A	914	LEU	2.3
1	C	410	ILE	2.3
1	C	7	ASP	2.3
1	C	152	GLU	2.2
1	B	988	PRO	2.2
1	C	832	ALA	2.2
1	B	989	LEU	2.2
1	B	832	ALA	2.2
1	C	6	ILE	2.2
1	A	418	ARG	2.2
1	A	515	TRP	2.2
1	C	414	GLU	2.2
1	C	535	LEU	2.2
1	B	670	ALA	2.2
1	C	831	ALA	2.2
1	B	420	MET	2.1
1	C	9	PRO	2.1
1	C	872	GLN	2.0
1	A	54	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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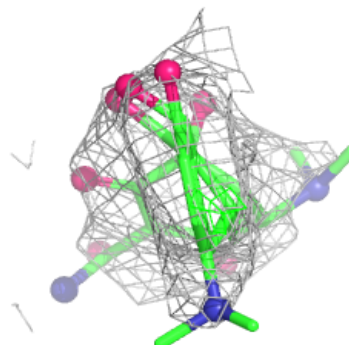
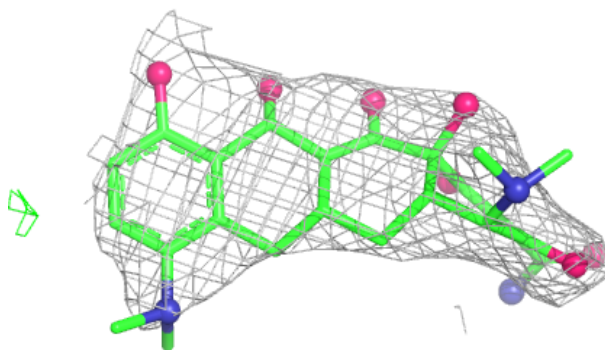
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MIY	A	2001	33/33	0.89	0.11	134,138,142,142	0
3	RFP	C	2002	59/59	0.90	0.13	131,136,139,140	0

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

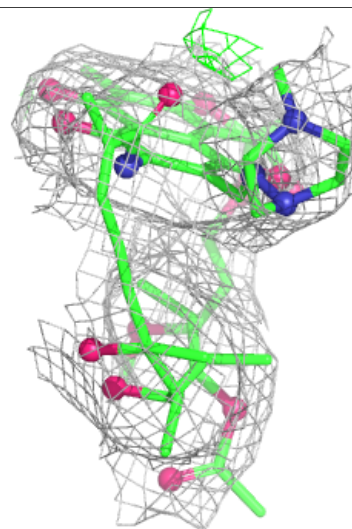
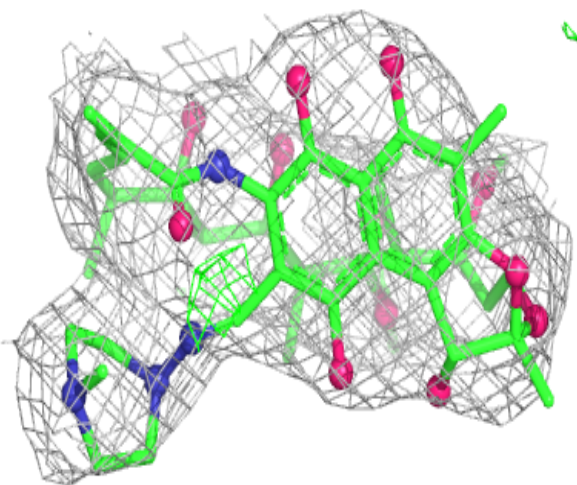
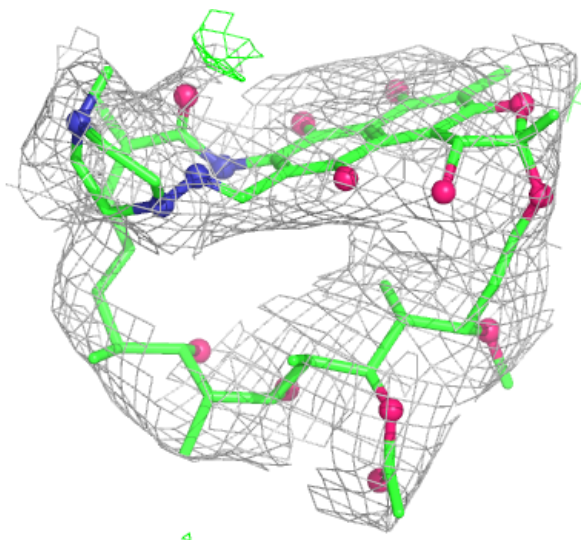
Electron density around MIY A 2001:

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



Electron density around RFP C 2002:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.