



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:03 am BST

PDB ID : 1IWO  
Title : Crystal structure of the SR Ca<sup>2+</sup>-ATPase in the absence of Ca<sup>2+</sup>  
Authors : Toyoshima, C.; Nomura, H.  
Deposited on : 2002-05-26  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

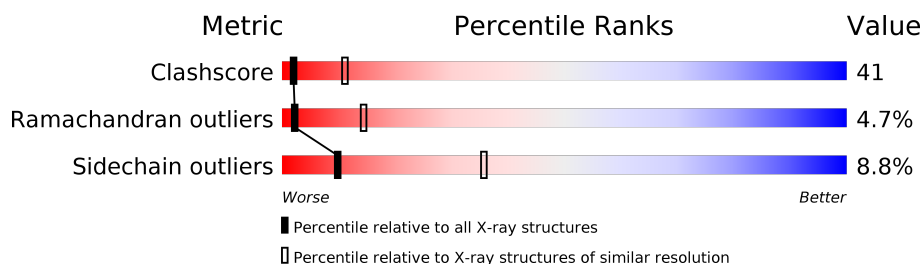
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	994	
1	B	994	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15434 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.

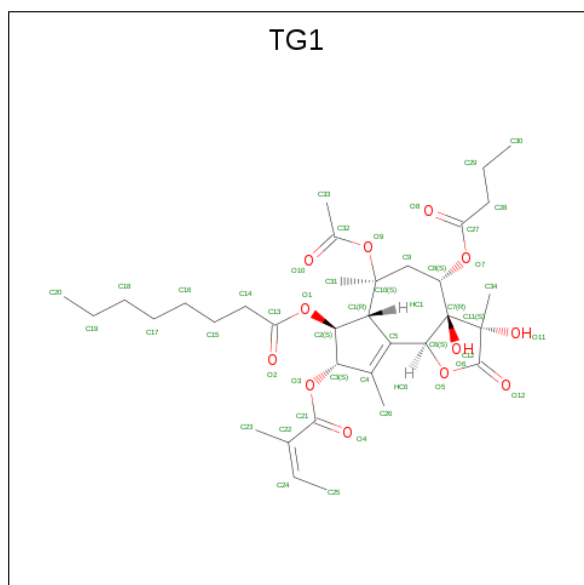
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			
1	B	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	ASP	SEE REMARK 999	UNP P04191
B	994	GLY	ASP	SEE REMARK 999	UNP P04191

- Molecule 2 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>12</sub>).



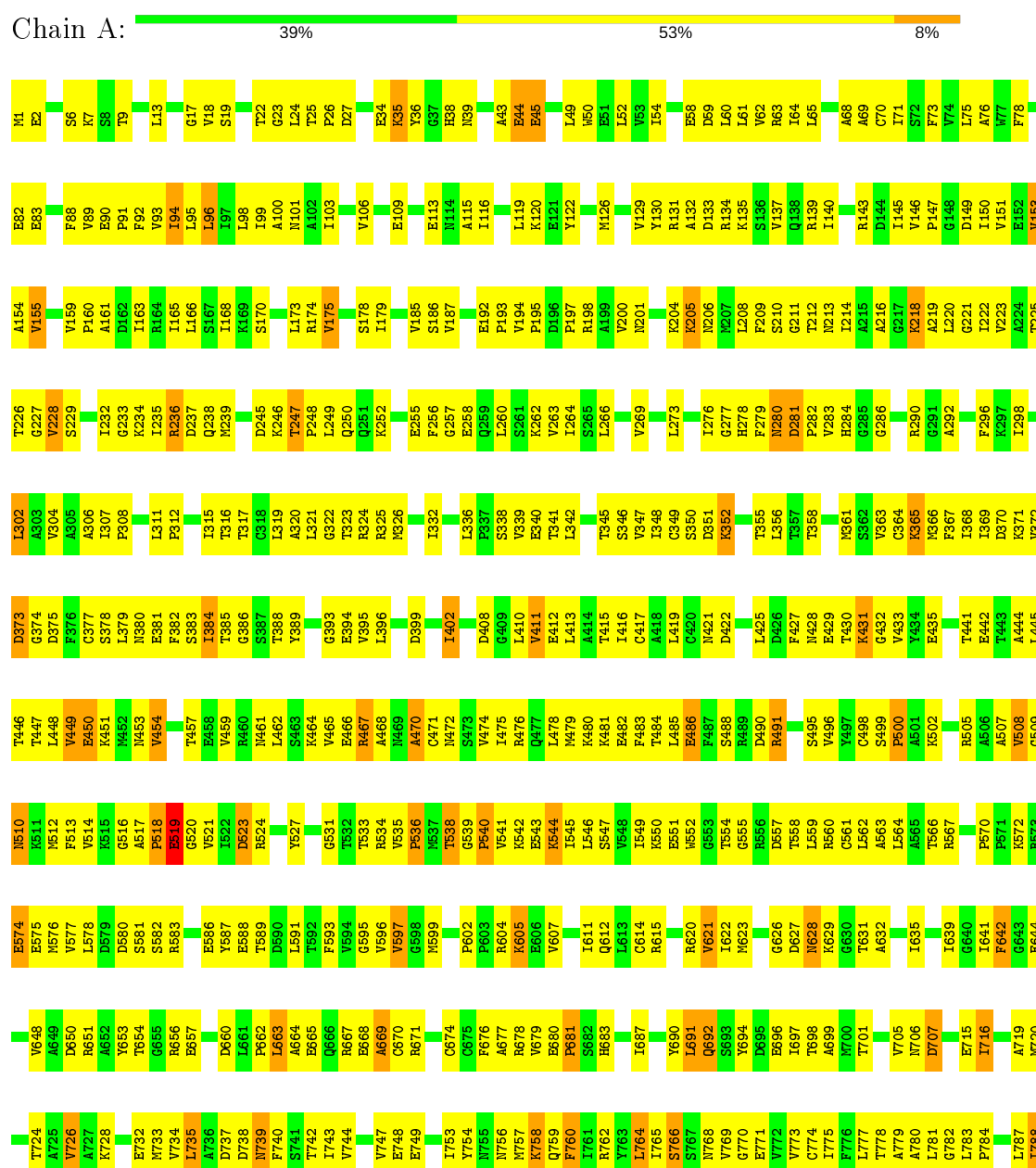
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 46	C 34	O 12	0	0
2	B	1	Total 46	C 34	O 12	0	0

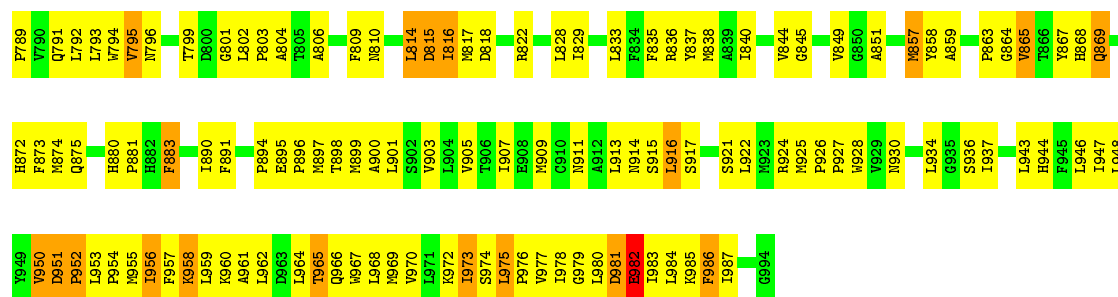
### 3 Residue-property plots

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

Note EDS was not executed.

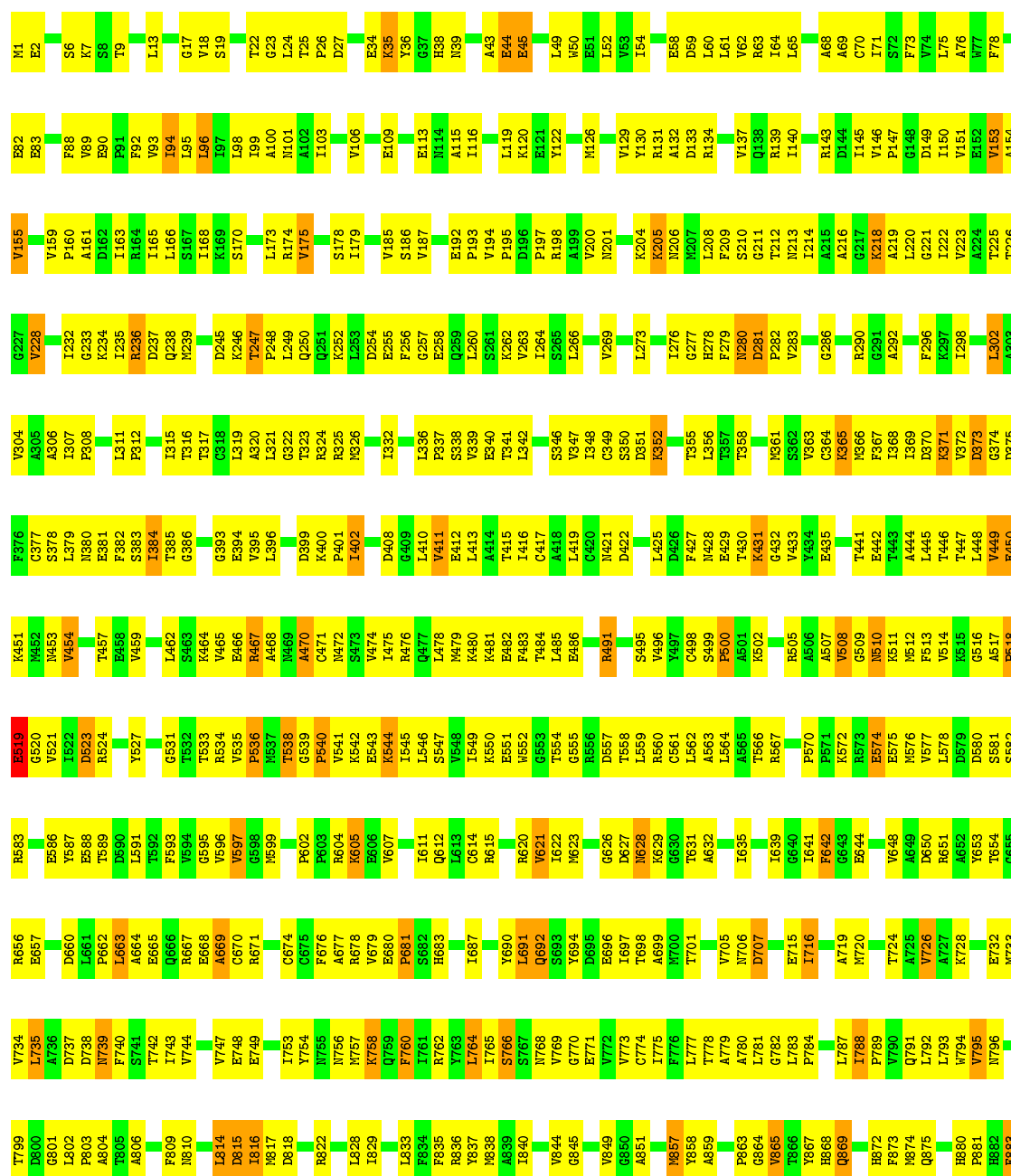
- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain B: 39% 52% 8%



P897	I890	P894	P895	P896	P897	M898	M899	A900	L901	S902	V903	L904	V905	T906	L907	P908	M909	C910	N911	A912	L913	N914	S915	L916	S917	S921	L922	R923	M924	M925	P926	P927	W928	W929	N930	L933	L934	G935	S936	I937	L943	H944	F945	L946	I947	L948	Y949	V950	D951	P952	L953	P954	M955	I956
I957	K958	L959	K960	A961	L962	D963	L964	T965	Q966	W967	L968	M969	V970	L971	K972	I973	S974	L975	P976	V977	I978	G979	L980	D981	E982	I983	L984	K985	F986	I987	G988	G989	G994																					

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.74 Å 71.74 Å 590.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.10	Depositor
% Data completeness (in resolution range)	95.7 (15.00-3.10)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TG1

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	0.44	1/7812 (0.0%)	0.67	2/10592 (0.0%)
1	B	0.44	1/7812 (0.0%)	0.67	2/10592 (0.0%)
All	All	0.44	2/15624 (0.0%)	0.67	4/21184 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	561	CYS	CB-SG	-5.93	1.72	1.81
1	A	561	CYS	CB-SG	-5.93	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	B	505	ARG	NE-CZ-NH2	7.21	123.90	120.30
1	A	508	VAL	CB-CA-C	-5.07	101.76	111.40
1	B	508	VAL	CB-CA-C	-5.07	101.76	111.40

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	7671	0	7764	634	0
1	B	7671	0	7764	633	0
2	A	46	0	50	5	0
2	B	46	0	50	5	0
All	All	15434	0	15628	1264	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 41.

All (1264) 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:958:LYS:HE3	1:A:958:LYS:HA	1.20	1.11
1:B:958:LYS:HE3	1:B:958:LYS:HA	1.20	1.09
1:B:201:ASN:HA	1:B:204:LYS:HD2	1.38	1.04
1:A:201:ASN:HA	1:A:204:LYS:HD2	1.38	1.02
1:B:411:VAL:HG13	1:B:454:VAL:HB	1.42	1.01
1:A:758:LYS:O	1:A:762:ARG:HG3	1.63	0.98
1:A:411:VAL:HG13	1:A:454:VAL:HB	1.42	0.97
1:B:538:THR:HB	1:B:540:PRO:HD2	1.45	0.96
1:A:538:THR:HB	1:A:540:PRO:HD2	1.45	0.96
1:B:758:LYS:O	1:B:762:ARG:HG3	1.63	0.96
1:B:247:THR:HG22	1:B:250:GLN:H	1.29	0.95
1:A:247:THR:HG22	1:A:250:GLN:H	1.29	0.94
1:B:368:ILE:HD13	1:B:410:LEU:HD23	1.51	0.93
1:B:788:ILE:HG22	1:B:789:PRO:HD2	1.51	0.91
1:A:788:ILE:HG22	1:A:789:PRO:HD2	1.51	0.90
1:A:368:ILE:HD13	1:A:410:LEU:HD23	1.51	0.90
1:B:583:ARG:O	1:B:586:GLU:HG2	1.72	0.89
1:A:583:ARG:O	1:A:586:GLU:HG2	1.72	0.89
1:B:481:LYS:HA	1:B:498:CYS:HB3	1.54	0.88
1:A:481:LYS:HA	1:A:498:CYS:HB3	1.54	0.88
1:B:232:ILE:H	1:B:232:ILE:HD12	1.38	0.88
1:A:232:ILE:H	1:A:232:ILE:HD12	1.38	0.88
1:B:174:ARG:HB2	1:B:216:ALA:HB3	1.56	0.87
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.56	0.86
1:B:1:MET:HG2	1:B:225:THR:HG22	1.57	0.86
1:B:262:LYS:NZ	1:B:266:LEU:HD21	1.91	0.85
1:A:604:ARG:HB3	1:A:607:VAL:HG13	1.57	0.85
1:A:100:ALA:HA	1:A:103:ILE:HD12	1.58	0.85
1:B:100:ALA:HA	1:B:103:ILE:HD12	1.58	0.85
1:A:984:LEU:O	1:A:987:ILE:HG22	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:ARG:HB3	1:B:607:VAL:HG13	1.57	0.84
1:B:984:LEU:O	1:B:987:ILE:HG22	1.77	0.84
1:A:1:MET:HG2	1:A:225:THR:HG22	1.57	0.84
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.60	0.84
1:A:13:LEU:HD23	1:A:222:ILE:HD12	1.58	0.84
1:A:262:LYS:NZ	1:A:266:LEU:HD21	1.91	0.84
1:A:89:VAL:O	1:A:93:VAL:HG23	1.77	0.84
1:A:383:SER:C	1:A:384:ILE:HD13	1.99	0.84
1:B:147:PRO:HA	1:B:223:VAL:HG12	1.60	0.84
1:B:383:SER:C	1:B:384:ILE:HD13	1.99	0.83
1:A:558:THR:HG21	1:A:635:ILE:HG12	1.61	0.83
1:B:89:VAL:O	1:B:93:VAL:HG23	1.77	0.83
1:B:13:LEU:HD23	1:B:222:ILE:HD12	1.58	0.83
1:B:558:THR:HG21	1:B:635:ILE:HG12	1.61	0.83
1:A:739:ASN:C	1:A:739:ASN:HD22	1.83	0.82
1:B:491:ARG:HG3	1:B:491:ARG:HH11	1.45	0.82
1:A:739:ASN:O	1:A:742:THR:HG22	1.80	0.82
1:A:873:PHE:HB2	1:A:875:GLN:HG3	1.62	0.82
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.45	0.82
1:B:873:PHE:HB2	1:B:875:GLN:HG3	1.62	0.82
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.60	0.81
1:A:563:ALA:O	1:A:564:LEU:HD23	1.80	0.81
1:B:739:ASN:O	1:B:742:THR:HG22	1.80	0.81
1:A:447:THR:HG22	1:A:451:LYS:HE3	1.63	0.81
1:B:447:THR:HG22	1:B:451:LYS:HE3	1.63	0.81
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.46	0.81
1:A:628:ASN:HD21	1:A:631:THR:H	1.28	0.81
1:A:890:ILE:H	1:A:890:ILE:HD12	1.46	0.81
1:B:260:LEU:HD11	1:B:306:ALA:HB1	1.60	0.81
1:B:739:ASN:HD22	1:B:739:ASN:C	1.83	0.80
1:B:563:ALA:O	1:B:564:LEU:HD23	1.80	0.80
1:A:961:ALA:HB1	1:A:966:GLN:HG2	1.64	0.80
1:A:557:ASP:O	1:A:559:LEU:HG	1.82	0.80
1:B:281:ASP:HB2	1:B:282:PRO:HD3	1.65	0.79
1:B:724:THR:O	1:B:728:LYS:HG3	1.82	0.79
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.64	0.79
1:B:890:ILE:HD12	1:B:890:ILE:H	1.46	0.79
1:B:557:ASP:O	1:B:559:LEU:HG	1.82	0.79
1:A:724:THR:O	1:A:728:LYS:HG3	1.82	0.78
1:B:129:VAL:HG12	1:B:151:VAL:HG12	1.65	0.78
1:B:680:GLU:HB3	1:B:681:PRO:HD2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:961:ALA:HB1	1:B:966:GLN:HG2	1.64	0.78
1:B:911:ASN:HA	1:B:914:ASN:HD22	1.46	0.78
1:B:628:ASN:HD21	1:B:631:THR:H	1.28	0.78
1:B:632:ALA:HA	1:B:635:ILE:HD12	1.66	0.78
1:B:153:VAL:HB	1:B:214:ILE:HG13	1.65	0.78
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.65	0.78
1:A:281:ASP:HB2	1:A:282:PRO:HD3	1.65	0.78
1:B:9:THR:HG23	1:B:166:LEU:HD22	1.67	0.77
1:B:52:LEU:HD23	1:B:106:VAL:HG13	1.67	0.77
1:A:153:VAL:HB	1:A:214:ILE:HG13	1.65	0.76
1:A:9:THR:HG23	1:A:166:LEU:HD22	1.67	0.76
1:A:52:LEU:HD23	1:A:106:VAL:HG13	1.67	0.75
1:A:632:ALA:HA	1:A:635:ILE:HD12	1.66	0.75
1:B:720:MET:HE3	1:B:738:ASP:HB3	1.68	0.75
1:B:705:VAL:HG13	1:B:726:VAL:HG21	1.69	0.75
1:A:802:LEU:HB3	1:A:936:SER:HB2	1.69	0.75
1:B:758:LYS:HG3	1:B:828:LEU:HD22	1.69	0.75
1:A:720:MET:HE3	1:A:738:ASP:HB3	1.68	0.75
1:B:958:LYS:HE3	1:B:958:LYS:CA	2.11	0.75
1:B:705:VAL:CG1	1:B:726:VAL:HG21	2.17	0.74
1:A:758:LYS:HG3	1:A:828:LEU:HD22	1.69	0.74
1:B:411:VAL:HG13	1:B:454:VAL:CB	2.18	0.74
1:B:947:ILE:HG22	1:B:953:LEU:HD13	1.69	0.74
1:A:851:ALA:HB1	1:A:903:VAL:HG21	1.70	0.74
1:B:802:LEU:HB3	1:B:936:SER:HB2	1.69	0.74
1:B:874:MET:HG2	1:B:891:PHE:CD2	2.23	0.74
1:A:366:MET:HE1	1:A:448:LEU:HD21	1.70	0.74
1:B:350:SER:HA	1:B:701:THR:HG21	1.70	0.74
1:A:319:LEU:HG	1:A:339:VAL:HG21	1.69	0.73
1:A:705:VAL:CG1	1:A:726:VAL:HG21	2.17	0.73
1:A:705:VAL:HG13	1:A:726:VAL:HG21	1.69	0.73
1:B:232:ILE:N	1:B:232:ILE:HD12	2.03	0.73
1:B:260:LEU:O	1:B:264:ILE:HG13	1.89	0.73
1:A:52:LEU:HG	1:A:106:VAL:HG22	1.70	0.73
1:A:260:LEU:O	1:A:264:ILE:HG13	1.89	0.73
1:A:232:ILE:N	1:A:232:ILE:HD12	2.03	0.73
1:A:350:SER:HA	1:A:701:THR:HG21	1.70	0.73
1:A:947:ILE:HG22	1:A:953:LEU:HD13	1.69	0.73
1:B:851:ALA:HB1	1:B:903:VAL:HG21	1.70	0.73
1:A:605:LYS:HD2	1:A:605:LYS:N	2.04	0.73
1:B:319:LEU:HG	1:B:339:VAL:HG21	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LYS:HZ2	1:B:266:LEU:HD21	1.54	0.72
1:B:52:LEU:HG	1:B:106:VAL:HG22	1.70	0.72
1:B:567:ARG:HH11	1:B:570:PRO:HA	1.55	0.72
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.54	0.72
1:B:683:HIS:O	1:B:687:ILE:HG13	1.88	0.72
1:B:605:LYS:HD2	1:B:605:LYS:N	2.04	0.72
1:B:628:ASN:ND2	1:B:631:THR:H	1.88	0.72
1:A:683:HIS:O	1:A:687:ILE:HG13	1.88	0.72
1:B:131:ARG:HG3	1:B:131:ARG:HH11	1.54	0.72
1:A:874:MET:HG2	1:A:891:PHE:CD2	2.23	0.72
1:A:979:GLY:O	1:A:983:ILE:HG12	1.90	0.72
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.72	0.71
1:A:628:ASN:ND2	1:A:631:THR:H	1.88	0.71
1:A:921:SER:HG	1:A:986:PHE:HD1	1.36	0.71
1:A:311:LEU:N	1:A:312:PRO:HD2	2.05	0.71
1:A:326:MET:HE1	1:A:339:VAL:HG12	1.72	0.71
1:B:921:SER:HG	1:B:986:PHE:HD1	1.37	0.71
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.72	0.71
1:B:756:ASN:OD1	1:B:810:ASN:HB2	1.91	0.71
1:B:865:VAL:HB	1:B:868:HIS:HB2	1.72	0.71
1:A:411:VAL:HG13	1:A:454:VAL:CB	2.18	0.71
1:A:958:LYS:HE3	1:A:958:LYS:CA	2.11	0.71
1:B:130:TYR:HB2	1:B:150:ILE:HG13	1.72	0.71
1:B:350:SER:HA	1:B:701:THR:CG2	2.21	0.71
1:A:567:ARG:HH11	1:A:570:PRO:HA	1.55	0.70
1:B:411:VAL:HA	1:B:454:VAL:HG11	1.72	0.70
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.27	0.70
1:A:130:TYR:HB2	1:A:150:ILE:HG13	1.72	0.70
1:A:967:TRP:O	1:A:970:VAL:HB	1.91	0.70
1:B:967:TRP:O	1:B:970:VAL:HB	1.91	0.70
1:B:50:TRP:CH2	1:B:54:ILE:HD11	2.27	0.70
1:A:350:SER:HA	1:A:701:THR:CG2	2.21	0.70
1:A:756:ASN:OD1	1:A:810:ASN:HB2	1.91	0.70
1:B:311:LEU:N	1:B:312:PRO:HD2	2.05	0.70
1:A:567:ARG:NH1	1:A:570:PRO:HA	2.07	0.70
1:B:476:ARG:HG3	1:B:476:ARG:HH11	1.56	0.70
1:A:535:VAL:HB	1:A:536:PRO:HD2	1.74	0.70
1:B:535:VAL:HB	1:B:536:PRO:HD2	1.74	0.70
1:B:370:ASP:HB3	1:B:378:SER:OG	1.92	0.70
1:B:351:ASP:H	1:B:701:THR:HG21	1.56	0.69
1:B:979:GLY:O	1:B:983:ILE:HG12	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ARG:HH12	1:B:588:GLU:CD	1.96	0.69
1:B:499:SER:HB2	1:B:500:PRO:HD2	1.74	0.69
1:B:567:ARG:NH1	1:B:570:PRO:HA	2.07	0.69
1:A:956:ILE:HG13	1:A:957:PHE:N	2.08	0.69
1:A:370:ASP:HB3	1:A:378:SER:OG	1.92	0.69
1:A:476:ARG:HG3	1:A:476:ARG:HH11	1.56	0.69
1:B:449:VAL:HG21	1:B:472:ASN:OD1	1.93	0.69
1:B:326:MET:HE1	1:B:339:VAL:HG12	1.75	0.69
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.23	0.69
1:A:351:ASP:H	1:A:701:THR:HG21	1.56	0.68
1:A:563:ALA:C	1:A:564:LEU:HD23	2.14	0.68
1:A:851:ALA:CB	1:A:903:VAL:HG21	2.24	0.68
1:A:499:SER:HB2	1:A:500:PRO:HD2	1.74	0.68
1:A:324:ARG:HD2	1:A:325:ARG:N	2.08	0.68
1:B:450:GLU:OE1	1:B:450:GLU:HA	1.94	0.68
1:A:631:THR:O	1:A:635:ILE:HG13	1.93	0.68
1:B:366:MET:HE1	1:B:448:LEU:HD21	1.75	0.68
1:A:491:ARG:HH12	1:A:588:GLU:CD	1.96	0.68
1:B:324:ARG:HD2	1:B:325:ARG:N	2.08	0.68
1:A:449:VAL:HG21	1:A:472:ASN:OD1	1.93	0.68
1:B:788:ILE:HG13	1:B:791:GLN:CD	2.14	0.68
1:B:802:LEU:HB2	1:B:803:PRO:HD3	1.76	0.68
1:A:367:PHE:CD2	1:A:379:LEU:HD13	2.29	0.68
1:A:232:ILE:H	1:A:232:ILE:CD1	2.07	0.68
1:A:26:PRO:HD3	1:A:133:ASP:HB3	1.76	0.68
1:A:262:LYS:HZ3	1:A:266:LEU:HD21	1.58	0.68
1:B:9:THR:HG23	1:B:166:LEU:CD2	2.24	0.68
1:A:450:GLU:OE1	1:A:450:GLU:HA	1.94	0.67
1:B:358:THR:OG1	1:B:602:PRO:HG2	1.94	0.67
1:A:352:LYS:HE2	1:A:635:ILE:HG21	1.75	0.67
1:B:324:ARG:HD2	1:B:324:ARG:C	2.15	0.67
1:B:922:LEU:HD23	1:B:927:PRO:HG3	1.77	0.67
1:B:499:SER:HB3	1:B:510:ASN:HD21	1.60	0.67
1:B:563:ALA:C	1:B:564:LEU:HD23	2.14	0.67
1:A:499:SER:HB3	1:A:510:ASN:ND2	2.10	0.67
1:A:720:MET:HB3	1:A:738:ASP:OD1	1.95	0.67
1:B:315:ILE:HD12	1:B:316:THR:N	2.09	0.67
1:B:631:THR:O	1:B:635:ILE:HG13	1.93	0.67
1:A:358:THR:OG1	1:A:602:PRO:HG2	1.94	0.67
1:B:781:LEU:O	1:B:783:LEU:N	2.28	0.67
1:B:967:TRP:CZ3	1:B:970:VAL:HG11	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:TRP:CZ3	1:A:970:VAL:HG11	2.30	0.67
1:B:352:LYS:HE2	1:B:635:ILE:HG21	1.75	0.67
1:B:368:ILE:HD13	1:B:410:LEU:CD2	2.23	0.67
1:B:956:ILE:HG13	1:B:957:PHE:N	2.08	0.67
1:A:319:LEU:HB3	1:A:336:LEU:HD12	1.76	0.67
1:A:788:ILE:HG13	1:A:791:GLN:CD	2.14	0.67
1:A:9:THR:HG23	1:A:166:LEU:CD2	2.24	0.67
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.76	0.67
1:A:315:ILE:HD12	1:A:316:THR:N	2.09	0.66
1:A:324:ARG:HD2	1:A:324:ARG:C	2.15	0.66
1:A:781:LEU:O	1:A:783:LEU:N	2.28	0.66
1:B:367:PHE:CD2	1:B:379:LEU:HD13	2.29	0.66
1:A:944:HIS:O	1:A:947:ILE:HG13	1.95	0.66
1:B:26:PRO:HD3	1:B:133:ASP:HB3	1.76	0.66
1:B:851:ALA:CB	1:B:903:VAL:HG21	2.24	0.66
1:A:130:TYR:HE2	1:A:137:VAL:HA	1.61	0.66
1:A:499:SER:HB3	1:A:510:ASN:HD21	1.60	0.66
1:B:944:HIS:O	1:B:947:ILE:HG13	1.96	0.66
1:A:140:ILE:HD11	1:A:145:ILE:HG12	1.77	0.66
1:A:19:SER:HB3	1:A:22:THR:OG1	1.95	0.66
1:A:622:ILE:HG23	1:A:674:CYS:HA	1.77	0.66
1:B:499:SER:HB3	1:B:510:ASN:ND2	2.10	0.66
1:B:863:PRO:HG2	1:B:890:ILE:HG21	1.76	0.66
1:B:278:HIS:HA	1:B:282:PRO:HD2	1.78	0.66
1:A:338:SER:HA	1:A:341:THR:HG22	1.78	0.66
1:A:447:THR:CG2	1:A:451:LYS:HE3	2.25	0.66
1:A:922:LEU:HD23	1:A:927:PRO:HG3	1.77	0.66
1:A:491:ARG:NH1	1:A:588:GLU:OE2	2.29	0.66
1:B:622:ILE:HG23	1:B:674:CYS:HA	1.77	0.66
1:B:642:PHE:CZ	1:B:648:VAL:HB	2.31	0.66
1:A:642:PHE:CZ	1:A:648:VAL:HB	2.31	0.66
1:A:863:PRO:HG2	1:A:890:ILE:HG21	1.76	0.66
1:B:140:ILE:HD11	1:B:145:ILE:HG12	1.77	0.66
1:B:232:ILE:H	1:B:232:ILE:CD1	2.07	0.66
1:A:262:LYS:HZ2	1:A:266:LEU:HD21	1.58	0.65
1:B:447:THR:CG2	1:B:451:LYS:HE3	2.26	0.65
1:B:19:SER:HB3	1:B:22:THR:OG1	1.95	0.65
1:B:319:LEU:HB3	1:B:336:LEU:HD12	1.76	0.65
1:B:517:ALA:HB1	1:B:519:GLU:OE1	1.97	0.65
1:A:373:ASP:O	1:A:375:ASP:N	2.30	0.65
1:B:720:MET:HB3	1:B:738:ASP:OD1	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:MET:HG2	1:A:891:PHE:HD2	1.61	0.65
1:B:373:ASP:O	1:B:375:ASP:N	2.30	0.65
1:B:396:LEU:HD12	1:B:396:LEU:O	1.97	0.65
1:B:342:LEU:HA	1:B:716:ILE:CD1	2.27	0.65
1:A:278:HIS:HA	1:A:282:PRO:HD2	1.78	0.65
1:B:367:PHE:HZ	1:B:545:ILE:HG23	1.62	0.65
1:A:396:LEU:O	1:A:396:LEU:HD12	1.97	0.65
1:A:483:PHE:HE2	1:A:485:LEU:HD21	1.62	0.65
1:A:863:PRO:O	1:A:865:VAL:N	2.30	0.65
1:B:130:TYR:HE2	1:B:137:VAL:HA	1.61	0.65
1:B:491:ARG:NH1	1:B:588:GLU:OE2	2.29	0.65
1:B:863:PRO:O	1:B:865:VAL:N	2.30	0.65
1:A:342:LEU:HA	1:A:716:ILE:CD1	2.27	0.65
1:B:338:SER:HA	1:B:341:THR:HG22	1.78	0.64
1:B:312:PRO:O	1:B:315:ILE:HG13	1.97	0.64
1:A:278:HIS:O	1:B:49:LEU:HB3	1.95	0.64
1:A:965:THR:HA	1:A:968:LEU:HD13	1.79	0.64
1:B:364:CYS:HA	1:B:384:ILE:HG12	1.79	0.64
1:A:663:LEU:H	1:A:663:LEU:HD12	1.63	0.64
1:B:663:LEU:HD12	1:B:663:LEU:H	1.63	0.64
1:B:483:PHE:HE2	1:B:485:LEU:HD21	1.62	0.64
1:B:572:LYS:HB3	1:B:574:GLU:OE2	1.98	0.64
1:A:312:PRO:O	1:A:315:ILE:HG13	1.97	0.64
1:A:367:PHE:HZ	1:A:545:ILE:HG23	1.62	0.64
1:B:874:MET:HG2	1:B:891:PHE:HD2	1.61	0.64
1:A:517:ALA:HB1	1:A:519:GLU:OE1	1.96	0.64
1:B:262:LYS:HZ3	1:B:266:LEU:HD21	1.63	0.64
1:A:408:ASP:O	1:A:411:VAL:HG23	1.99	0.63
1:B:965:THR:HA	1:B:968:LEU:HD13	1.79	0.63
1:B:366:MET:HG3	1:B:382:PHE:HB2	1.79	0.63
1:A:572:LYS:HB3	1:A:574:GLU:OE2	1.98	0.63
1:A:668:GLU:O	1:A:671:ARG:HG2	1.98	0.63
1:A:844:VAL:CG1	1:A:907:ILE:HG21	2.29	0.63
1:A:364:CYS:HA	1:A:384:ILE:HG12	1.79	0.63
1:B:396:LEU:HD13	1:B:399:ASP:HA	1.81	0.63
1:B:739:ASN:HD22	1:B:740:PHE:N	1.96	0.63
1:B:895:GLU:N	1:B:896:PRO:HD2	2.14	0.63
1:A:396:LEU:HD13	1:A:399:ASP:HA	1.81	0.62
1:A:873:PHE:HD1	1:A:875:GLN:H	1.46	0.62
1:B:668:GLU:O	1:B:671:ARG:HG2	1.98	0.62
1:A:366:MET:HG3	1:A:382:PHE:HB2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:PRO:O	1:A:899:MET:HB2	1.99	0.62
1:B:873:PHE:HD1	1:B:875:GLN:H	1.46	0.62
1:A:377:CYS:HB3	1:A:541:VAL:HG22	1.81	0.62
1:B:402:ILE:HD13	1:B:402:ILE:H	1.65	0.62
1:B:377:CYS:HB3	1:B:541:VAL:HG22	1.81	0.62
1:A:739:ASN:HD22	1:A:740:PHE:N	1.96	0.62
1:B:408:ASP:O	1:B:411:VAL:HG23	1.99	0.62
1:B:737:ASP:OD2	1:B:739:ASN:HB3	1.99	0.62
1:B:39:ASN:OD1	1:B:226:THR:HB	2.00	0.62
1:B:662:PRO:HD2	1:B:665:GLU:OE2	1.99	0.62
1:B:355:THR:HG22	1:B:740:PHE:HB2	1.82	0.62
1:B:896:PRO:O	1:B:899:MET:HB2	1.98	0.62
1:A:59:ASP:O	1:A:62:VAL:HG22	2.00	0.62
1:A:662:PRO:HD2	1:A:665:GLU:OE2	1.99	0.62
1:A:737:ASP:OD2	1:A:739:ASN:HB3	2.00	0.62
1:B:814:LEU:CD2	1:B:815:ASP:H	2.13	0.62
1:A:342:LEU:HD12	1:A:716:ILE:HD13	1.82	0.62
1:B:951:ASP:HB2	1:B:952:PRO:HD3	1.80	0.62
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.80	0.62
1:A:355:THR:HG22	1:A:740:PHE:HB2	1.82	0.61
1:B:342:LEU:HD12	1:B:716:ILE:HD13	1.82	0.61
1:A:39:ASN:OD1	1:A:226:THR:HB	2.00	0.61
1:A:739:ASN:C	1:A:739:ASN:ND2	2.54	0.61
1:A:765:ILE:HD11	1:A:829:ILE:HD12	1.83	0.61
1:A:895:GLU:N	1:A:896:PRO:HD2	2.14	0.61
1:B:50:TRP:CZ3	1:B:54:ILE:HD11	2.35	0.61
1:A:542:LYS:HE3	1:A:546:LEU:HD11	1.82	0.61
1:B:765:ILE:HD11	1:B:829:ILE:HD12	1.83	0.61
1:A:950:VAL:O	1:A:954:PRO:HD2	2.01	0.61
1:B:950:VAL:O	1:B:954:PRO:HD2	2.01	0.61
1:B:263:VAL:O	1:B:266:LEU:HB2	2.01	0.61
1:B:264:ILE:HG23	1:B:302:LEU:HD12	1.82	0.61
1:B:844:VAL:CG1	1:B:907:ILE:HG21	2.29	0.61
1:A:50:TRP:CZ3	1:A:54:ILE:HD11	2.36	0.60
1:B:491:ARG:NH1	1:B:491:ARG:HG3	2.16	0.60
1:A:298:ILE:O	1:A:302:LEU:HB2	2.01	0.60
1:A:457:THR:O	1:A:459:VAL:HG13	2.01	0.60
1:A:792:LEU:O	1:A:795:VAL:HB	2.02	0.60
1:B:298:ILE:O	1:B:302:LEU:HB2	2.01	0.60
1:B:792:LEU:O	1:B:795:VAL:HB	2.01	0.60
1:A:402:ILE:HD13	1:A:402:ILE:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:LEU:CD2	1:A:815:ASP:H	2.13	0.60
1:A:947:ILE:O	1:A:947:ILE:HD12	2.02	0.60
1:A:130:TYR:CE2	1:A:137:VAL:HA	2.36	0.60
1:A:366:MET:O	1:A:366:MET:HG3	2.01	0.60
1:B:59:ASP:O	1:B:62:VAL:HG22	2.00	0.60
1:B:457:THR:O	1:B:459:VAL:HG13	2.01	0.60
1:B:947:ILE:O	1:B:947:ILE:HD12	2.02	0.60
1:A:264:ILE:HG23	1:A:302:LEU:HD12	1.82	0.60
1:A:131:ARG:NH1	1:A:131:ARG:HG3	2.17	0.59
1:A:355:THR:HA	1:A:738:ASP:O	2.02	0.59
1:B:384:ILE:N	1:B:384:ILE:HD13	2.17	0.59
1:B:542:LYS:HE3	1:B:546:LEU:HD11	1.82	0.59
1:A:263:VAL:O	1:A:266:LEU:HB2	2.01	0.59
1:B:130:TYR:CE2	1:B:137:VAL:HA	2.36	0.59
1:A:384:ILE:N	1:A:384:ILE:HD13	2.17	0.59
1:A:502:LYS:O	1:A:502:LYS:HG3	2.02	0.59
1:B:319:LEU:HG	1:B:339:VAL:CG2	2.32	0.59
1:B:417:CYS:O	1:B:421:ASN:HB2	2.03	0.59
1:B:968:LEU:HD12	1:B:968:LEU:H	1.67	0.59
1:A:916:LEU:HB2	1:A:925:MET:SD	2.42	0.59
1:B:52:LEU:CD2	1:B:106:VAL:HG13	2.33	0.59
1:A:735:LEU:HD13	1:A:742:THR:CG2	2.33	0.59
1:A:968:LEU:HD12	1:A:968:LEU:H	1.67	0.59
1:B:441:THR:HG21	1:B:560:ARG:NH1	2.18	0.59
1:B:628:ASN:HD21	1:B:631:THR:N	1.99	0.59
1:B:863:PRO:CG	1:B:890:ILE:HG21	2.32	0.59
1:B:975:LEU:H	1:B:975:LEU:HD22	1.67	0.59
1:A:441:THR:HG21	1:A:560:ARG:NH1	2.18	0.59
1:A:519:GLU:H	1:A:519:GLU:CD	2.05	0.59
1:A:605:LYS:HD2	1:A:605:LYS:H	1.68	0.59
1:A:880:HIS:N	1:A:881:PRO:HD2	2.18	0.59
1:A:970:VAL:O	1:A:973:ILE:HG22	2.03	0.59
1:B:880:HIS:N	1:B:881:PRO:HD2	2.18	0.59
1:A:417:CYS:O	1:A:421:ASN:HB2	2.03	0.59
1:B:519:GLU:H	1:B:519:GLU:CD	2.05	0.59
1:A:863:PRO:CG	1:A:890:ILE:HG21	2.32	0.59
1:B:351:ASP:N	1:B:701:THR:HG21	2.18	0.59
1:A:499:SER:CB	1:A:510:ASN:ND2	2.66	0.58
1:B:367:PHE:CE2	1:B:379:LEU:HD13	2.38	0.58
1:B:413:LEU:HD22	1:B:564:LEU:HD12	1.85	0.58
1:B:735:LEU:HD13	1:B:742:THR:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:VAL:O	1:A:545:ILE:HG13	2.03	0.58
1:A:975:LEU:HD22	1:A:975:LEU:H	1.67	0.58
1:B:126:MET:SD	1:B:139:ARG:HD3	2.43	0.58
1:B:366:MET:HG3	1:B:366:MET:O	2.01	0.58
1:B:482:GLU:HG2	1:B:498:CYS:HA	1.86	0.58
1:B:355:THR:HA	1:B:738:ASP:O	2.02	0.58
1:A:366:MET:CE	1:A:448:LEU:HD21	2.34	0.58
1:A:482:GLU:HG2	1:A:498:CYS:HA	1.86	0.58
1:A:801:GLY:O	1:A:804:ALA:HB3	2.04	0.58
1:B:366:MET:CE	1:B:448:LEU:HD21	2.34	0.58
1:B:502:LYS:O	1:B:502:LYS:HG3	2.02	0.58
1:B:844:VAL:HG12	1:B:907:ILE:HG21	1.86	0.58
1:A:356:LEU:CD2	1:A:623:MET:HG3	2.33	0.58
1:B:958:LYS:HA	1:B:958:LYS:CE	2.09	0.58
1:A:130:TYR:HE2	1:A:137:VAL:CA	2.16	0.58
1:B:247:THR:HG23	1:B:340:GLU:OE1	2.04	0.58
1:B:366:MET:HB3	1:B:597:VAL:HG12	1.84	0.58
1:A:757:MET:HA	1:A:760:PHE:CE2	2.39	0.58
1:B:499:SER:CB	1:B:510:ASN:ND2	2.66	0.58
1:A:52:LEU:CD2	1:A:106:VAL:HG13	2.33	0.58
1:B:739:ASN:C	1:B:739:ASN:ND2	2.54	0.58
1:A:247:THR:HG23	1:A:340:GLU:OE1	2.04	0.58
1:A:248:PRO:O	1:A:252:LYS:HG2	2.04	0.58
1:A:319:LEU:HG	1:A:339:VAL:CG2	2.32	0.58
1:B:18:VAL:HG12	1:B:19:SER:N	2.19	0.58
1:A:126:MET:SD	1:A:139:ARG:HD3	2.43	0.58
1:A:351:ASP:N	1:A:701:THR:HG21	2.18	0.58
1:A:367:PHE:CE2	1:A:379:LEU:HD13	2.38	0.58
1:A:527:TYR:HB3	1:A:534:ARG:HD3	1.85	0.58
1:B:541:VAL:O	1:B:545:ILE:HG13	2.03	0.58
1:B:916:LEU:HB2	1:B:925:MET:SD	2.42	0.58
1:A:628:ASN:HD21	1:A:631:THR:N	1.99	0.57
1:A:947:ILE:O	1:A:948:LEU:HD12	2.04	0.57
1:B:970:VAL:O	1:B:973:ILE:HG22	2.03	0.57
1:A:366:MET:HB3	1:A:597:VAL:HG12	1.84	0.57
1:A:810:ASN:HD21	1:A:916:LEU:HA	1.69	0.57
1:B:342:LEU:HA	1:B:716:ILE:HD13	1.85	0.57
1:B:757:MET:HA	1:B:760:PHE:CE2	2.39	0.57
1:A:336:LEU:O	1:A:339:VAL:HG22	2.04	0.57
1:A:491:ARG:HG3	1:A:491:ARG:NH1	2.16	0.57
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:PRO:HB2	1:A:959:LEU:H	1.69	0.57
1:B:130:TYR:HE2	1:B:137:VAL:CA	2.16	0.57
1:B:527:TYR:HB3	1:B:534:ARG:HD3	1.85	0.57
1:A:346:SER:OG	1:A:696:GLU:HG2	2.04	0.57
1:A:676:PHE:CE1	1:A:687:ILE:HD13	2.40	0.57
1:A:765:ILE:O	1:A:769:VAL:HG23	2.05	0.57
1:B:209:PHE:O	1:B:212:THR:HB	2.05	0.57
1:B:346:SER:OG	1:B:696:GLU:HG2	2.04	0.57
1:B:615:ARG:NH1	1:B:620:ARG:HA	2.20	0.57
1:B:676:PHE:CE1	1:B:687:ILE:HD13	2.40	0.57
1:A:276:ILE:HG22	1:A:279:PHE:HB3	1.86	0.57
1:B:629:LYS:HB2	1:B:654:THR:HG22	1.86	0.57
1:B:911:ASN:HA	1:B:914:ASN:ND2	2.18	0.57
1:B:248:PRO:O	1:B:252:LYS:HG2	2.04	0.57
1:B:801:GLY:O	1:B:804:ALA:HB3	2.04	0.57
1:B:758:LYS:HZ1	1:B:822:ARG:HE	1.52	0.57
1:B:947:ILE:O	1:B:948:LEU:HD12	2.04	0.57
1:A:212:THR:CG2	1:A:213:ASN:N	2.68	0.57
1:B:356:LEU:CD2	1:B:623:MET:HG3	2.33	0.57
1:A:629:LYS:HB2	1:A:654:THR:HG22	1.86	0.57
1:A:844:VAL:HG12	1:A:907:ILE:HG21	1.86	0.57
1:B:833:LEU:HG	1:B:837:TYR:CE2	2.40	0.57
1:B:967:TRP:CE3	1:B:970:VAL:HG11	2.40	0.57
1:A:13:LEU:CD2	1:A:222:ILE:HD12	2.33	0.57
1:A:342:LEU:HA	1:A:716:ILE:HD13	1.85	0.57
1:B:276:ILE:HG22	1:B:279:PHE:HB3	1.86	0.57
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.85	0.56
1:A:18:VAL:HG12	1:A:19:SER:N	2.19	0.56
1:A:161:ALA:HA	1:A:210:SER:HB2	1.88	0.56
1:A:539:GLY:O	1:A:543:GLU:HG2	2.05	0.56
1:A:833:LEU:HG	1:A:837:TYR:HE2	1.70	0.56
1:B:212:THR:CG2	1:B:213:ASN:N	2.68	0.56
1:A:814:LEU:HD22	1:A:815:ASP:H	1.70	0.56
1:B:161:ALA:HA	1:B:210:SER:HB2	1.88	0.56
1:B:336:LEU:O	1:B:339:VAL:HG22	2.04	0.56
1:B:914:ASN:HB3	1:B:981:ASP:OD2	2.05	0.56
1:A:209:PHE:O	1:A:212:THR:HB	2.05	0.56
1:B:605:LYS:H	1:B:605:LYS:HD2	1.68	0.56
1:A:143:ARG:HG2	1:A:143:ARG:HH11	1.70	0.56
1:A:205:LYS:NZ	1:A:205:LYS:HB3	2.20	0.56
1:B:367:PHE:CZ	1:B:545:ILE:HG23	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:894:PRO:HB2	1:B:959:LEU:H	1.69	0.56
1:A:833:LEU:HG	1:A:837:TYR:CE2	2.40	0.56
1:A:901:LEU:O	1:A:905:VAL:HG23	2.06	0.56
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.70	0.56
1:B:791:GLN:O	1:B:795:VAL:HG23	2.06	0.56
1:B:833:LEU:HG	1:B:837:TYR:HE2	1.70	0.56
1:A:416:ILE:HD11	1:A:566:THR:HG23	1.87	0.56
1:A:615:ARG:NH1	1:A:620:ARG:HA	2.20	0.56
1:A:791:GLN:O	1:A:795:VAL:HG23	2.06	0.56
1:B:765:ILE:O	1:B:769:VAL:HG23	2.05	0.56
1:B:774:CYS:SG	1:B:787:LEU:HD12	2.45	0.56
1:B:76:ALA:O	1:B:88:PHE:HE2	1.89	0.56
1:B:13:LEU:CD2	1:B:222:ILE:HD12	2.33	0.56
1:B:810:ASN:HD21	1:B:916:LEU:HA	1.70	0.56
1:A:967:TRP:CE3	1:A:970:VAL:HG11	2.40	0.56
1:A:749:GLU:O	1:A:753:ILE:HG12	2.06	0.55
1:A:794:TRP:HH2	1:A:943:LEU:HB3	1.72	0.55
1:B:18:VAL:HG13	1:B:24:LEU:HD23	1.87	0.55
1:B:205:LYS:NZ	1:B:205:LYS:HB3	2.20	0.55
1:A:76:ALA:O	1:A:88:PHE:HE2	1.89	0.55
1:A:844:VAL:HG12	1:A:907:ILE:HD13	1.89	0.55
1:B:416:ILE:HD11	1:B:566:THR:HG23	1.87	0.55
1:A:147:PRO:HA	1:A:223:VAL:CG1	2.35	0.55
1:A:367:PHE:CZ	1:A:545:ILE:HG23	2.41	0.55
1:A:576:MET:HE3	1:A:587:TYR:HB3	1.89	0.55
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.05	0.55
1:B:539:GLY:O	1:B:543:GLU:HG2	2.05	0.55
1:A:921:SER:OG	1:A:986:PHE:HD1	1.89	0.55
1:B:298:ILE:C	1:B:298:ILE:HD12	2.27	0.55
1:B:322:GLY:O	1:B:325:ARG:HB3	2.07	0.55
1:B:844:VAL:HG12	1:B:907:ILE:HD13	1.89	0.55
1:B:901:LEU:O	1:B:905:VAL:HG23	2.06	0.55
1:A:18:VAL:HG13	1:A:24:LEU:HD23	1.87	0.55
1:A:836:ARG:O	1:A:840:ILE:HG12	2.07	0.55
1:A:322:GLY:O	1:A:325:ARG:HB3	2.07	0.55
1:B:363:VAL:HB	1:B:448:LEU:HD13	1.89	0.55
1:B:576:MET:HE3	1:B:587:TYR:HB3	1.88	0.55
1:B:749:GLU:O	1:B:753:ILE:HG12	2.06	0.55
1:A:7:LYS:HA	1:A:7:LYS:HE2	1.89	0.55
1:B:586:GLU:O	1:B:589:THR:HG22	2.07	0.55
1:A:284:HIS:CE1	1:B:45:GLU:HB3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:ARG:O	1:B:840:ILE:HG12	2.07	0.55
1:A:325:ARG:NH1	1:A:753:ILE:HD11	2.22	0.54
1:A:735:LEU:HD22	1:A:742:THR:HG23	1.89	0.54
1:B:814:LEU:HD22	1:B:815:ASP:H	1.70	0.54
1:A:586:GLU:O	1:A:589:THR:HG22	2.07	0.54
1:A:911:ASN:HA	1:A:914:ASN:ND2	2.18	0.54
1:B:131:ARG:HG3	1:B:131:ARG:NH1	2.17	0.54
1:B:668:GLU:OE1	1:B:671:ARG:HD3	2.07	0.54
1:B:325:ARG:NH1	1:B:753:ILE:HD11	2.22	0.54
1:B:773:VAL:HB	1:B:845:GLY:HA3	1.88	0.54
1:A:428:ASN:HB2	1:A:435:GLU:CG	2.38	0.54
1:A:773:VAL:HB	1:A:845:GLY:HA3	1.88	0.54
1:B:192:GLU:HG3	1:B:193:PRO:HD2	1.90	0.54
1:B:428:ASN:HB2	1:B:435:GLU:CG	2.38	0.54
1:B:899:MET:O	1:B:903:VAL:HG23	2.07	0.54
1:A:315:ILE:O	1:A:319:LEU:HD13	2.08	0.54
1:B:364:CYS:O	1:B:383:SER:HA	2.07	0.54
1:A:298:ILE:C	1:A:298:ILE:HD12	2.27	0.54
1:A:748:GLU:HG3	1:A:817:MET:SD	2.47	0.54
1:B:748:GLU:HG3	1:B:817:MET:SD	2.47	0.54
1:A:260:LEU:HD13	2:A:1001:TG1:H252	1.89	0.54
1:A:476:ARG:HG3	1:A:476:ARG:NH1	2.23	0.54
1:A:894:PRO:O	1:A:898:THR:HG22	2.08	0.54
1:A:1:MET:HG2	1:A:225:THR:CG2	2.34	0.54
1:A:668:GLU:OE1	1:A:671:ARG:HD3	2.07	0.54
1:B:315:ILE:O	1:B:319:LEU:HD13	2.08	0.54
1:B:794:TRP:HH2	1:B:943:LEU:HB3	1.72	0.54
1:B:977:VAL:HG13	1:B:978:ILE:N	2.23	0.54
1:A:315:ILE:HD12	1:A:315:ILE:C	2.29	0.53
1:A:363:VAL:HB	1:A:448:LEU:HD13	1.89	0.53
1:A:967:TRP:HZ3	1:A:970:VAL:HG11	1.73	0.53
1:B:735:LEU:HD22	1:B:742:THR:HG23	1.89	0.53
1:B:894:PRO:O	1:B:898:THR:HG22	2.08	0.53
1:A:192:GLU:HG3	1:A:193:PRO:HD2	1.90	0.53
1:B:50:TRP:O	1:B:54:ILE:HG12	2.08	0.53
1:B:962:LEU:O	1:B:966:GLN:HB3	2.08	0.53
1:B:921:SER:OG	1:B:986:PHE:HD1	1.89	0.53
1:A:364:CYS:O	1:A:383:SER:HA	2.07	0.53
1:A:962:LEU:O	1:A:966:GLN:HB3	2.08	0.53
1:B:762:ARG:O	1:B:766:SER:HB3	2.08	0.53
1:A:622:ILE:HG23	1:A:674:CYS:CA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:MET:O	1:A:903:VAL:HG23	2.07	0.53
1:B:116:ILE:HA	1:B:119:LEU:HD23	1.91	0.53
1:B:1:MET:HG2	1:B:225:THR:CG2	2.34	0.53
1:A:50:TRP:O	1:A:54:ILE:HG12	2.08	0.53
1:A:762:ARG:O	1:A:766:SER:HB3	2.08	0.53
1:B:476:ARG:HG3	1:B:476:ARG:NH1	2.23	0.53
1:B:622:ILE:HG23	1:B:674:CYS:CA	2.39	0.53
1:A:558:THR:O	1:A:558:THR:HG22	2.08	0.53
1:A:863:PRO:O	1:A:865:VAL:HG13	2.09	0.53
1:B:558:THR:HG22	1:B:558:THR:O	2.08	0.53
1:B:1:MET:HA	1:B:225:THR:HG22	1.91	0.53
1:A:868:HIS:O	1:A:869:GLN:HB2	2.09	0.53
1:A:977:VAL:HG13	1:A:978:ILE:N	2.24	0.53
1:B:7:LYS:HA	1:B:7:LYS:HE2	1.89	0.53
1:B:868:HIS:O	1:B:869:GLN:HB2	2.09	0.53
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.39	0.53
1:B:260:LEU:HD13	2:B:1002:TG1:H252	1.89	0.53
1:A:1:MET:HA	1:A:225:THR:HG22	1.91	0.52
1:A:903:VAL:O	1:A:907:ILE:HG13	2.09	0.52
1:A:924:ARG:HA	1:A:924:ARG:NE	2.24	0.52
1:B:777:LEU:O	1:B:780:ALA:N	2.41	0.52
1:A:382:PHE:CZ	1:A:410:LEU:HD11	2.45	0.52
1:B:412:GLU:HA	1:B:415:THR:OG1	2.10	0.52
1:B:671:ARG:HD2	1:B:694:TYR:CZ	2.45	0.52
1:B:924:ARG:NE	1:B:924:ARG:HA	2.24	0.52
1:A:462:LEU:HD22	1:A:466:GLU:OE1	2.10	0.52
1:A:627:ASP:O	1:A:677:ALA:HB1	2.10	0.52
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.45	0.52
1:A:769:VAL:HA	2:A:1001:TG1:H231	1.91	0.52
1:B:495:SER:CB	1:B:588:GLU:OE1	2.58	0.52
1:B:628:ASN:HD21	1:B:631:THR:CB	2.23	0.52
1:B:627:ASP:O	1:B:677:ALA:HB1	2.10	0.52
1:B:705:VAL:HG12	1:B:726:VAL:HG21	1.92	0.52
1:B:758:LYS:NZ	1:B:822:ARG:HE	2.07	0.52
1:B:863:PRO:O	1:B:865:VAL:HG13	2.09	0.52
1:A:366:MET:HE2	1:A:448:LEU:HD11	1.91	0.52
1:A:758:LYS:NZ	1:A:822:ARG:HE	2.07	0.52
1:A:857:MET:SD	1:A:867:TYR:HA	2.50	0.52
1:B:596:VAL:HG12	1:B:597:VAL:N	2.24	0.52
1:B:611:ILE:HD12	1:B:641:ILE:HD11	1.92	0.52
1:B:769:VAL:HA	2:B:1002:TG1:H231	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:903:VAL:O	1:B:907:ILE:HG13	2.09	0.52
1:A:495:SER:CB	1:A:588:GLU:OE1	2.58	0.52
1:A:49:LEU:O	1:A:49:LEU:HD23	2.10	0.52
1:A:355:THR:OG1	1:A:720:MET:CE	2.58	0.52
1:B:24:LEU:HG	1:B:149:ASP:HA	1.92	0.52
1:B:315:ILE:C	1:B:315:ILE:HD12	2.29	0.52
1:B:366:MET:HE2	1:B:448:LEU:HD11	1.92	0.52
1:B:671:ARG:HB3	1:B:694:TYR:CE1	2.45	0.52
1:B:770:GLY:HA3	1:B:844:VAL:CG2	2.39	0.52
1:A:412:GLU:HA	1:A:415:THR:OG1	2.10	0.52
1:A:924:ARG:C	1:A:926:PRO:HD3	2.30	0.52
1:B:705:VAL:HG12	1:B:726:VAL:HG11	1.91	0.52
1:B:235:ILE:HD11	1:B:706:ASN:HA	1.92	0.52
1:B:715:GLU:C	1:B:716:ILE:HG13	2.30	0.52
1:B:865:VAL:HB	1:B:868:HIS:CB	2.39	0.52
1:A:18:VAL:HG12	1:A:19:SER:H	1.74	0.52
1:A:173:LEU:HD12	1:A:216:ALA:O	2.10	0.52
1:A:628:ASN:HD21	1:A:631:THR:CB	2.23	0.52
1:A:705:VAL:HG12	1:A:726:VAL:HG11	1.91	0.52
1:A:235:ILE:HD11	1:A:706:ASN:HA	1.92	0.52
1:B:18:VAL:HG12	1:B:19:SER:H	1.74	0.52
1:B:382:PHE:CZ	1:B:410:LEU:HD11	2.45	0.52
1:B:924:ARG:C	1:B:926:PRO:HD3	2.30	0.52
1:A:596:VAL:HG12	1:A:597:VAL:N	2.24	0.52
1:A:958:LYS:HA	1:A:958:LYS:CE	2.09	0.51
1:B:495:SER:HB3	1:B:588:GLU:OE1	2.11	0.51
1:A:116:ILE:HA	1:A:119:LEU:HD23	1.91	0.51
1:A:810:ASN:HA	1:A:930:ASN:HD22	1.76	0.51
1:B:49:LEU:O	1:B:49:LEU:HD23	2.10	0.51
1:A:247:THR:HG23	1:A:249:LEU:H	1.75	0.51
1:A:361:MET:HG2	1:A:441:THR:HA	1.92	0.51
1:A:671:ARG:HB3	1:A:694:TYR:CE1	2.45	0.51
1:A:865:VAL:HB	1:A:868:HIS:CB	2.39	0.51
1:B:155:VAL:HA	1:B:214:ILE:O	2.10	0.51
1:B:247:THR:HG23	1:B:249:LEU:H	1.75	0.51
1:B:355:THR:OG1	1:B:720:MET:CE	2.58	0.51
1:B:621:VAL:HG13	1:B:641:ILE:HD12	1.93	0.51
1:A:198:ARG:HH11	1:A:198:ARG:HG2	1.76	0.51
1:A:611:ILE:HD12	1:A:641:ILE:HD11	1.92	0.51
1:A:705:VAL:C	1:A:707:ASP:H	2.13	0.51
1:A:760:PHE:C	1:A:760:PHE:CD1	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HG	1:A:149:ASP:HA	1.92	0.51
1:A:715:GLU:C	1:A:716:ILE:HG13	2.30	0.51
1:B:71:ILE:HG22	1:B:75:LEU:HD13	1.92	0.51
1:A:155:VAL:HA	1:A:214:ILE:O	2.10	0.51
1:A:466:GLU:C	1:A:468:ALA:H	2.14	0.51
1:A:680:GLU:CB	1:A:681:PRO:HD2	2.38	0.51
1:B:173:LEU:HD12	1:B:216:ALA:O	2.10	0.51
1:B:462:LEU:HD22	1:B:466:GLU:OE1	2.10	0.51
1:B:614:CYS:SG	1:B:744:VAL:HG22	2.51	0.51
1:B:760:PHE:C	1:B:760:PHE:CD1	2.84	0.51
1:B:857:MET:SD	1:B:867:TYR:HA	2.50	0.51
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.93	0.51
1:A:179:ILE:O	1:A:705:VAL:HG22	2.11	0.51
1:B:179:ILE:O	1:B:705:VAL:HG22	2.11	0.51
1:A:794:TRP:CH2	1:A:943:LEU:HB3	2.46	0.51
1:B:133:ASP:O	1:B:134:ARG:HG3	2.11	0.51
1:B:24:LEU:HD12	1:B:149:ASP:HB3	1.93	0.51
1:B:466:GLU:C	1:B:468:ALA:H	2.14	0.51
1:A:133:ASP:O	1:A:134:ARG:HG3	2.11	0.51
1:A:621:VAL:HG13	1:A:641:ILE:HD12	1.93	0.51
1:A:614:CYS:SG	1:A:744:VAL:HG22	2.51	0.51
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.46	0.51
1:B:198:ARG:HH11	1:B:198:ARG:HG2	1.76	0.51
1:B:969:MET:O	1:B:973:ILE:HB	2.11	0.51
1:A:61:LEU:HD22	1:A:307:ILE:CD1	2.41	0.51
1:A:342:LEU:HA	1:A:716:ILE:HD11	1.92	0.51
1:A:705:VAL:HG12	1:A:726:VAL:HG21	1.92	0.51
1:B:370:ASP:HB2	1:B:379:LEU:O	2.11	0.51
1:B:794:TRP:CH2	1:B:943:LEU:HB3	2.46	0.51
1:A:201:ASN:HB3	1:A:209:PHE:CZ	2.46	0.50
1:A:754:TYR:O	1:A:754:TYR:CD1	2.64	0.50
1:A:836:ARG:HG2	1:A:836:ARG:HH11	1.77	0.50
1:A:987:ILE:HG12	1:A:987:ILE:O	2.12	0.50
1:B:705:VAL:C	1:B:707:ASP:H	2.13	0.50
1:B:925:MET:HE3	1:B:985:LYS:HZ3	1.75	0.50
1:A:25:THR:O	1:A:27:ASP:N	2.44	0.50
1:A:278:HIS:O	1:B:49:LEU:CB	2.59	0.50
1:A:577:VAL:HG11	1:A:580:ASP:OD2	2.11	0.50
1:B:228:VAL:HA	1:B:233:GLY:HA3	1.93	0.50
1:B:361:MET:HG2	1:B:441:THR:HA	1.92	0.50
1:B:957:PHE:O	1:B:958:LYS:NZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLU:O	1:B:45:GLU:HG3	2.12	0.50
1:B:754:TYR:O	1:B:754:TYR:CD1	2.65	0.50
1:B:810:ASN:HA	1:B:930:ASN:HD22	1.75	0.50
1:B:987:ILE:HG12	1:B:987:ILE:O	2.12	0.50
1:A:777:LEU:O	1:A:780:ALA:N	2.41	0.50
1:A:957:PHE:O	1:A:958:LYS:NZ	2.42	0.50
1:B:281:ASP:HB2	1:B:282:PRO:CD	2.35	0.50
1:B:444:ALA:HB3	1:B:599:MET:HE1	1.92	0.50
1:B:61:LEU:HD22	1:B:307:ILE:CD1	2.41	0.50
1:B:69:ALA:O	1:B:73:PHE:HB2	2.12	0.50
1:A:71:ILE:HG22	1:A:75:LEU:HD13	1.92	0.50
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.76	0.50
1:A:863:PRO:HG2	1:A:890:ILE:CG2	2.42	0.50
1:B:201:ASN:HB3	1:B:209:PHE:CZ	2.46	0.50
1:B:235:ILE:CD1	1:B:706:ASN:HA	2.42	0.50
1:B:342:LEU:HA	1:B:716:ILE:HD11	1.92	0.50
1:B:593:PHE:HZ	1:B:596:VAL:HG23	1.77	0.50
1:B:65:LEU:O	1:B:68:ALA:HB3	2.12	0.50
1:B:795:VAL:HA	1:B:799:THR:OG1	2.12	0.50
1:A:680:GLU:HB3	1:A:681:PRO:CD	2.39	0.50
1:A:69:ALA:O	1:A:73:PHE:HB2	2.12	0.50
1:A:969:MET:O	1:A:973:ILE:HB	2.11	0.50
1:B:25:THR:O	1:B:27:ASP:N	2.44	0.50
1:A:235:ILE:CD1	1:A:706:ASN:HA	2.42	0.50
1:A:44:GLU:O	1:A:45:GLU:HG3	2.12	0.50
1:A:546:LEU:O	1:A:549:ILE:N	2.45	0.50
1:B:470:ALA:O	1:B:474:VAL:HG23	2.12	0.50
1:B:546:LEU:O	1:B:549:ILE:N	2.45	0.50
1:B:758:LYS:HG3	1:B:828:LEU:CD2	2.41	0.50
1:A:320:ALA:O	1:A:323:THR:HB	2.12	0.50
1:A:412:GLU:O	1:A:415:THR:N	2.45	0.50
1:A:500:PRO:HD3	1:A:509:GLY:O	2.12	0.50
1:A:639:ILE:HG13	1:A:641:ILE:HG12	1.93	0.50
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.27	0.50
1:B:320:ALA:O	1:B:323:THR:HB	2.12	0.50
1:B:639:ILE:HG13	1:B:641:ILE:HG12	1.93	0.50
1:B:771:GLU:O	1:B:774:CYS:HB3	2.12	0.50
1:B:950:VAL:O	1:B:952:PRO:HD2	2.12	0.50
1:A:495:SER:HB3	1:A:588:GLU:OE1	2.10	0.49
1:A:795:VAL:HA	1:A:799:THR:OG1	2.11	0.49
1:B:500:PRO:HD3	1:B:509:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:MET:HG2	1:B:891:PHE:CE2	2.47	0.49
1:B:967:TRP:HZ3	1:B:970:VAL:HG11	1.73	0.49
1:A:278:HIS:HA	1:A:282:PRO:CD	2.42	0.49
1:A:281:ASP:HB2	1:A:282:PRO:CD	2.35	0.49
1:A:442:GLU:O	1:A:445:LEU:N	2.46	0.49
1:A:470:ALA:O	1:A:474:VAL:HG23	2.12	0.49
1:A:518:PRO:HA	1:A:563:ALA:HB2	1.94	0.49
1:A:631:THR:HG22	1:A:635:ILE:HD11	1.93	0.49
1:B:278:HIS:HA	1:B:282:PRO:CD	2.42	0.49
1:B:442:GLU:O	1:B:445:LEU:N	2.46	0.49
1:B:513:PHE:HD1	1:B:566:THR:HG22	1.76	0.49
1:B:631:THR:HG22	1:B:635:ILE:HD11	1.93	0.49
1:B:769:VAL:HG21	2:B:1002:TG1:H332	1.95	0.49
1:A:228:VAL:HA	1:A:233:GLY:HA3	1.93	0.49
1:A:771:GLU:O	1:A:774:CYS:HB3	2.12	0.49
1:A:874:MET:HG2	1:A:891:PHE:CE2	2.47	0.49
1:B:577:VAL:HG11	1:B:580:ASP:OD2	2.11	0.49
1:A:370:ASP:HB2	1:A:379:LEU:O	2.11	0.49
1:A:734:VAL:O	1:A:734:VAL:HG12	2.13	0.49
1:B:70:CYS:O	1:B:71:ILE:C	2.51	0.49
1:B:926:PRO:HB3	1:B:928:TRP:CE2	2.46	0.49
1:A:546:LEU:O	1:A:549:ILE:HB	2.13	0.49
1:A:95:LEU:O	1:A:99:ILE:HG13	2.13	0.49
1:B:147:PRO:HA	1:B:223:VAL:CG1	2.35	0.49
1:B:159:VAL:HG23	1:B:212:THR:O	2.12	0.49
1:B:552:TRP:HB3	1:B:559:LEU:HD12	1.94	0.49
1:A:527:TYR:HD1	1:A:536:PRO:HA	1.77	0.49
1:A:593:PHE:HZ	1:A:596:VAL:HG23	1.77	0.49
1:A:65:LEU:O	1:A:68:ALA:HB3	2.12	0.49
1:B:836:ARG:HH11	1:B:836:ARG:HG2	1.77	0.49
1:A:154:ALA:CB	1:A:218:LYS:HB2	2.43	0.49
1:A:159:VAL:HG23	1:A:212:THR:O	2.12	0.49
1:A:444:ALA:HB3	1:A:599:MET:CE	2.43	0.49
1:A:680:GLU:HB2	1:A:683:HIS:CE1	2.48	0.49
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.95	0.49
1:B:653:TYR:O	1:B:676:PHE:HA	2.13	0.49
1:A:952:PRO:O	1:A:955:MET:HB3	2.13	0.49
1:B:680:GLU:HB2	1:B:683:HIS:CE1	2.48	0.49
1:B:863:PRO:HG2	1:B:890:ILE:CG2	2.42	0.49
1:B:115:ALA:HB3	1:B:239:MET:HE1	1.95	0.49
1:B:869:GLN:HB3	1:B:872:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:HG21	1:B:140:ILE:HD13	1.94	0.49
1:B:154:ALA:CB	1:B:218:LYS:HB2	2.43	0.48
1:B:444:ALA:HB3	1:B:599:MET:CE	2.43	0.48
1:B:527:TYR:HD1	1:B:536:PRO:HA	1.77	0.48
1:B:546:LEU:O	1:B:549:ILE:HB	2.13	0.48
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.27	0.48
1:A:232:ILE:N	1:A:232:ILE:CD1	2.72	0.48
1:A:366:MET:CE	1:A:448:LEU:HD11	2.43	0.48
1:A:444:ALA:HB3	1:A:599:MET:HE1	1.94	0.48
1:A:70:CYS:O	1:A:71:ILE:C	2.51	0.48
1:A:765:ILE:HD13	2:A:1001:TG1:H292	1.95	0.48
1:B:317:THR:O	1:B:321:LEU:HG	2.13	0.48
1:B:518:PRO:HA	1:B:563:ALA:HB2	1.94	0.48
1:A:799:THR:O	1:A:909:MET:HE3	2.13	0.48
1:A:917:SER:N	1:A:925:MET:HE2	2.28	0.48
1:A:950:VAL:O	1:A:952:PRO:HD2	2.12	0.48
1:B:23:GLY:O	1:B:132:ALA:HB2	2.14	0.48
1:B:350:SER:HB3	1:B:356:LEU:HD11	1.96	0.48
1:B:412:GLU:O	1:B:415:THR:N	2.45	0.48
1:B:952:PRO:O	1:B:955:MET:HB3	2.12	0.48
1:B:95:LEU:O	1:B:99:ILE:HG13	2.13	0.48
1:A:433:VAL:HG13	1:A:435:GLU:OE2	2.14	0.48
1:A:774:CYS:HA	1:A:845:GLY:O	2.13	0.48
1:B:49:LEU:C	1:B:49:LEU:HD23	2.34	0.48
1:B:628:ASN:ND2	1:B:631:THR:N	2.60	0.48
1:B:775:ILE:HG22	1:B:775:ILE:O	2.13	0.48
1:B:777:LEU:HB2	1:B:849:VAL:HG21	1.95	0.48
1:A:317:THR:O	1:A:321:LEU:HG	2.13	0.48
1:A:481:LYS:HE2	1:A:496:VAL:HG21	1.96	0.48
1:A:836:ARG:HG2	1:A:836:ARG:NH1	2.29	0.48
1:A:959:LEU:HG	1:A:960:LYS:N	2.28	0.48
1:A:769:VAL:HG21	2:A:1001:TG1:H332	1.95	0.48
1:A:311:LEU:N	1:A:312:PRO:CD	2.76	0.48
1:A:552:TRP:HB3	1:A:559:LEU:HD12	1.94	0.48
1:A:653:TYR:O	1:A:676:PHE:HA	2.13	0.48
1:B:366:MET:CE	1:B:448:LEU:HD11	2.43	0.48
1:B:593:PHE:C	1:B:593:PHE:CD1	2.87	0.48
1:B:959:LEU:HG	1:B:960:LYS:N	2.28	0.48
1:A:129:VAL:HG21	1:A:140:ILE:HD13	1.94	0.48
1:A:355:THR:OG1	1:A:720:MET:HE2	2.14	0.48
1:B:137:VAL:O	1:B:137:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:SER:CB	1:B:510:ASN:HD21	2.27	0.48
1:A:137:VAL:O	1:A:137:VAL:HG13	2.13	0.48
1:A:915:SER:C	1:A:917:SER:H	2.17	0.48
1:B:372:VAL:HG12	1:B:373:ASP:N	2.29	0.48
1:B:433:VAL:HG13	1:B:435:GLU:OE2	2.14	0.48
1:B:915:SER:C	1:B:917:SER:H	2.17	0.48
1:A:372:VAL:HG12	1:A:373:ASP:N	2.29	0.48
1:B:481:LYS:HE2	1:B:496:VAL:HG21	1.96	0.48
1:B:774:CYS:HA	1:B:845:GLY:O	2.13	0.48
1:A:544:LYS:HA	1:A:544:LYS:HE2	1.96	0.47
1:A:698:THR:HG22	1:A:699:ALA:N	2.29	0.47
1:A:775:ILE:HG22	1:A:775:ILE:O	2.13	0.47
1:A:897:MET:SD	1:A:958:LYS:HD3	2.54	0.47
1:A:427:PHE:HB3	1:A:465:VAL:HG22	1.96	0.47
1:B:304:VAL:HG21	1:B:789:PRO:HA	1.96	0.47
1:B:680:GLU:HB3	1:B:681:PRO:CD	2.39	0.47
1:A:968:LEU:HD12	1:A:968:LEU:N	2.29	0.47
1:A:427:PHE:CD2	1:A:464:LYS:HB3	2.49	0.47
1:A:869:GLN:HB3	1:A:872:HIS:CD2	2.48	0.47
1:A:966:GLN:HA	1:A:966:GLN:NE2	2.29	0.47
1:B:844:VAL:HG11	1:B:907:ILE:HG21	1.96	0.47
1:A:115:ALA:HB3	1:A:239:MET:HE1	1.95	0.47
1:A:304:VAL:HG21	1:A:789:PRO:HA	1.96	0.47
1:A:350:SER:HB3	1:A:356:LEU:HD11	1.96	0.47
1:A:626:GLY:O	1:A:678:ARG:NE	2.45	0.47
1:A:777:LEU:O	1:A:779:ALA:N	2.48	0.47
1:A:844:VAL:HG11	1:A:907:ILE:HG21	1.96	0.47
1:B:269:VAL:O	1:B:273:LEU:HG	2.14	0.47
1:B:430:THR:HB	1:B:431:LYS:HD2	1.97	0.47
1:B:734:VAL:HG12	1:B:734:VAL:O	2.13	0.47
1:A:869:GLN:HB3	1:A:872:HIS:HD2	1.80	0.47
1:B:166:LEU:HG	1:B:221:GLY:HA2	1.97	0.47
1:B:255:GLU:O	1:B:258:GLU:HB2	2.15	0.47
1:B:427:PHE:CD2	1:B:464:LYS:HB3	2.49	0.47
1:B:604:ARG:O	1:B:607:VAL:HG22	2.15	0.47
1:B:836:ARG:NH1	1:B:836:ARG:HG2	2.29	0.47
1:B:946:LEU:O	1:B:953:LEU:HD12	2.15	0.47
1:A:277:GLY:O	1:A:280:ASN:N	2.48	0.47
1:A:312:PRO:HA	1:A:315:ILE:HG13	1.96	0.47
1:A:428:ASN:O	1:A:432:GLY:HA2	2.15	0.47
1:A:49:LEU:HD23	1:A:49:LEU:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:ASN:ND2	1:A:631:THR:N	2.60	0.47
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.97	0.47
1:A:98:LEU:O	1:A:101:ASN:HB3	2.14	0.47
1:B:765:ILE:HD13	2:B:1002:TG1:H292	1.95	0.47
1:B:544:LYS:HE2	1:B:544:LYS:HA	1.96	0.47
1:A:269:VAL:O	1:A:273:LEU:HG	2.14	0.47
1:A:956:ILE:HD11	1:A:957:PHE:CZ	2.50	0.47
1:B:427:PHE:HB3	1:B:465:VAL:HG22	1.96	0.47
1:B:966:GLN:HA	1:B:966:GLN:NE2	2.29	0.47
1:A:255:GLU:O	1:A:258:GLU:HB2	2.15	0.47
1:A:365:LYS:HB2	1:A:552:TRP:CZ3	2.50	0.47
1:A:593:PHE:C	1:A:593:PHE:CD1	2.87	0.47
1:A:92:PHE:O	1:A:96:LEU:HB2	2.15	0.47
1:B:98:LEU:O	1:B:101:ASN:HB3	2.14	0.47
1:B:192:GLU:CG	1:B:193:PRO:HD2	2.45	0.47
1:B:278:HIS:HA	1:B:282:PRO:CG	2.44	0.47
1:B:311:LEU:N	1:B:312:PRO:CD	2.77	0.47
1:B:347:VAL:HG12	1:B:348:ILE:N	2.30	0.47
1:B:719:ALA:O	1:B:734:VAL:HA	2.15	0.47
1:B:917:SER:N	1:B:925:MET:HE2	2.30	0.47
1:B:968:LEU:HD12	1:B:968:LEU:N	2.29	0.47
1:A:23:GLY:O	1:A:132:ALA:HB2	2.14	0.47
1:A:946:LEU:O	1:A:953:LEU:HD12	2.15	0.47
1:B:365:LYS:HB2	1:B:552:TRP:CZ3	2.50	0.47
1:B:620:ARG:HH22	1:B:671:ARG:HA	1.80	0.47
1:B:628:ASN:HD22	1:B:628:ASN:N	2.13	0.47
1:B:835:PHE:O	1:B:838:MET:HB3	2.15	0.47
1:B:92:PHE:O	1:B:96:LEU:HB2	2.15	0.47
1:A:342:LEU:O	1:A:345:THR:OG1	2.24	0.46
1:A:499:SER:CB	1:A:510:ASN:HD21	2.27	0.46
1:A:620:ARG:HH22	1:A:671:ARG:HA	1.80	0.46
1:A:754:TYR:HA	1:A:757:MET:HE2	1.98	0.46
1:A:308:PRO:HA	1:A:768:ASN:HD21	1.80	0.46
1:A:869:GLN:O	1:A:872:HIS:HB2	2.15	0.46
1:B:130:TYR:HB2	1:B:150:ILE:CG1	2.44	0.46
1:B:308:PRO:HA	1:B:768:ASN:HD21	1.80	0.46
1:B:338:SER:C	1:B:340:GLU:N	2.67	0.46
1:B:428:ASN:O	1:B:432:GLY:HA2	2.15	0.46
1:B:777:LEU:O	1:B:779:ALA:N	2.48	0.46
1:B:925:MET:SD	1:B:925:MET:O	2.73	0.46
1:B:956:ILE:HD11	1:B:957:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:MET:SD	1:B:958:LYS:HD3	2.54	0.46
1:A:352:LYS:HE3	1:A:635:ILE:HD13	1.97	0.46
1:A:604:ARG:O	1:A:607:VAL:HG22	2.15	0.46
1:A:835:PHE:O	1:A:838:MET:HB3	2.15	0.46
1:B:312:PRO:HA	1:B:315:ILE:HG13	1.96	0.46
1:B:425:LEU:HD13	1:B:446:THR:HG21	1.96	0.46
1:A:119:LEU:HD12	1:A:232:ILE:CG2	2.46	0.46
1:A:35:LYS:HD3	1:A:35:LYS:C	2.36	0.46
1:A:514:VAL:HG21	1:A:591:LEU:HD22	1.97	0.46
1:A:868:HIS:O	1:A:869:GLN:CB	2.64	0.46
1:B:508:VAL:HG12	1:B:509:GLY:N	2.30	0.46
1:A:338:SER:C	1:A:340:GLU:N	2.67	0.46
1:B:462:LEU:HB3	1:B:466:GLU:CB	2.46	0.46
1:B:869:GLN:HB3	1:B:872:HIS:HD2	1.80	0.46
1:B:895:GLU:N	1:B:896:PRO:CD	2.78	0.46
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.97	0.46
1:A:192:GLU:CG	1:A:193:PRO:HD2	2.45	0.46
1:A:168:ILE:HA	1:A:219:ALA:CB	2.46	0.46
1:A:278:HIS:HA	1:A:282:PRO:CG	2.44	0.46
1:A:462:LEU:HB3	1:A:466:GLU:CB	2.46	0.46
1:A:508:VAL:HG12	1:A:509:GLY:N	2.30	0.46
1:A:690:TYR:C	1:A:692:GLN:N	2.69	0.46
1:A:925:MET:SD	1:A:925:MET:O	2.73	0.46
1:B:119:LEU:HD12	1:B:232:ILE:CG2	2.46	0.46
1:B:626:GLY:O	1:B:678:ARG:NE	2.45	0.46
1:A:719:ALA:O	1:A:734:VAL:HA	2.15	0.46
1:A:810:ASN:ND2	1:A:916:LEU:HA	2.30	0.46
1:B:154:ALA:O	1:B:214:ILE:HB	2.16	0.46
1:B:168:ILE:HA	1:B:219:ALA:CB	2.46	0.46
1:B:499:SER:CB	1:B:500:PRO:HD2	2.44	0.46
1:B:580:ASP:O	1:B:583:ARG:N	2.45	0.46
1:A:425:LEU:HD13	1:A:446:THR:HG21	1.96	0.46
1:A:408:ASP:HB2	1:A:531:GLY:HA2	1.97	0.46
1:A:628:ASN:HD22	1:A:628:ASN:N	2.13	0.46
1:A:924:ARG:O	1:A:926:PRO:HD3	2.16	0.46
1:B:550:LYS:O	1:B:551:GLU:C	2.54	0.46
1:B:90:GLU:OE1	1:B:789:PRO:HG3	2.16	0.46
1:B:810:ASN:ND2	1:B:916:LEU:HA	2.30	0.46
1:A:154:ALA:O	1:A:214:ILE:HB	2.16	0.46
1:A:166:LEU:HG	1:A:221:GLY:HA2	1.97	0.46
1:A:430:THR:HB	1:A:431:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LYS:O	1:B:238:GLN:HG3	2.16	0.46
1:B:290:ARG:C	1:B:292:ALA:H	2.20	0.46
1:B:408:ASP:HB2	1:B:531:GLY:HA2	1.97	0.46
1:B:441:THR:HG22	1:B:441:THR:O	2.16	0.46
1:B:754:TYR:OH	1:B:828:LEU:HD21	2.16	0.46
1:B:957:PHE:O	1:B:958:LYS:CE	2.64	0.46
1:A:234:LYS:O	1:A:238:GLN:HG3	2.16	0.46
1:A:347:VAL:HG12	1:A:348:ILE:N	2.30	0.45
1:A:654:THR:HA	1:A:677:ALA:O	2.17	0.45
1:B:43:ALA:HB2	1:B:120:LYS:NZ	2.31	0.45
1:B:25:THR:C	1:B:27:ASP:N	2.70	0.45
1:B:514:VAL:HG21	1:B:591:LEU:HD22	1.97	0.45
1:B:347:VAL:HG13	1:B:620:ARG:HB3	1.98	0.45
1:A:174:ARG:HD3	1:A:186:SER:OG	2.16	0.45
1:B:212:THR:HG22	1:B:213:ASN:N	2.31	0.45
1:B:277:GLY:O	1:B:280:ASN:N	2.48	0.45
1:B:278:HIS:CA	1:B:282:PRO:HD2	2.45	0.45
1:B:698:THR:HG22	1:B:699:ALA:N	2.29	0.45
1:B:857:MET:C	1:B:859:ALA:H	2.20	0.45
1:A:100:ALA:HA	1:A:103:ILE:CD1	2.40	0.45
1:A:146:VAL:HG23	1:A:147:PRO:O	2.17	0.45
1:A:441:THR:HG22	1:A:441:THR:O	2.16	0.45
1:A:550:LYS:O	1:A:551:GLU:C	2.54	0.45
1:A:754:TYR:OH	1:A:828:LEU:HD21	2.16	0.45
1:B:175:VAL:HG12	1:B:213:ASN:O	2.16	0.45
1:B:516:GLY:O	1:B:563:ALA:N	2.49	0.45
1:B:533:THR:HG22	1:B:534:ARG:N	2.31	0.45
1:B:816:ILE:CG2	1:B:817:MET:N	2.79	0.45
1:B:868:HIS:O	1:B:869:GLN:CB	2.64	0.45
1:B:869:GLN:O	1:B:872:HIS:HB2	2.15	0.45
1:B:924:ARG:O	1:B:926:PRO:HD3	2.16	0.45
1:A:43:ALA:HB2	1:A:120:LYS:NZ	2.31	0.45
1:A:890:ILE:H	1:A:890:ILE:CD1	2.24	0.45
1:B:146:VAL:HG23	1:B:147:PRO:O	2.17	0.45
1:B:174:ARG:HD3	1:B:186:SER:OG	2.16	0.45
1:B:35:LYS:C	1:B:35:LYS:HD3	2.36	0.45
1:B:393:GLY:O	1:B:394:GLU:HG3	2.17	0.45
1:B:628:ASN:ND2	1:B:628:ASN:O	2.49	0.45
1:A:533:THR:HG22	1:A:534:ARG:N	2.31	0.45
1:A:551:GLU:O	1:A:555:GLY:N	2.44	0.45
1:A:697:ILE:HA	1:A:715:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:MET:C	1:A:859:ALA:H	2.20	0.45
1:A:784:PRO:HG3	1:A:874:MET:HE3	1.99	0.45
1:A:957:PHE:O	1:A:958:LYS:CE	2.64	0.45
1:A:968:LEU:H	1:A:968:LEU:CD1	2.29	0.45
1:B:679:VAL:HG13	1:B:679:VAL:O	2.16	0.45
1:B:799:THR:O	1:B:909:MET:HE3	2.16	0.45
1:A:347:VAL:HG13	1:A:620:ARG:HB3	1.98	0.45
1:A:628:ASN:ND2	1:A:628:ASN:O	2.49	0.45
1:A:873:PHE:HD1	1:A:875:GLN:N	2.12	0.45
1:B:475:ILE:HA	1:B:478:LEU:HD13	1.99	0.45
1:B:580:ASP:O	1:B:582:SER:N	2.50	0.45
1:B:697:ILE:HA	1:B:715:GLU:HG2	1.99	0.45
1:B:791:GLN:O	1:B:792:LEU:C	2.55	0.45
1:B:968:LEU:CD1	1:B:968:LEU:H	2.29	0.45
1:A:175:VAL:HG12	1:A:213:ASN:O	2.16	0.45
1:A:428:ASN:HB2	1:A:435:GLU:HG3	1.99	0.45
1:A:580:ASP:O	1:A:582:SER:N	2.50	0.45
1:A:246:LYS:HB3	1:A:250:GLN:HE21	1.82	0.45
1:A:816:ILE:CG2	1:A:817:MET:N	2.80	0.45
1:A:90:GLU:OE1	1:A:789:PRO:HG3	2.16	0.45
1:B:447:THR:O	1:B:451:LYS:HG3	2.17	0.45
1:B:352:LYS:HE3	1:B:635:ILE:HD13	1.97	0.45
1:B:654:THR:HA	1:B:677:ALA:O	2.17	0.45
1:A:212:THR:HG22	1:A:213:ASN:N	2.31	0.45
1:A:393:GLY:O	1:A:394:GLU:HG3	2.17	0.45
1:A:419:LEU:CD1	1:A:479:MET:HB2	2.46	0.45
1:A:679:VAL:HG13	1:A:679:VAL:O	2.16	0.45
1:A:791:GLN:HE22	1:A:897:MET:HB3	1.82	0.45
1:B:419:LEU:CD1	1:B:479:MET:HB2	2.46	0.45
1:B:784:PRO:HG3	1:B:874:MET:HE3	1.99	0.45
1:A:179:ILE:HD13	1:A:211:GLY:O	2.18	0.45
1:A:290:ARG:C	1:A:292:ALA:H	2.20	0.45
1:A:380:ASN:OD1	1:A:382:PHE:CE1	2.69	0.45
1:A:416:ILE:O	1:A:417:CYS:C	2.56	0.45
1:B:236:ARG:NH1	1:B:237:ASP:OD2	2.50	0.45
1:B:380:ASN:OD1	1:B:382:PHE:CE1	2.69	0.45
1:B:52:LEU:HD11	1:B:109:GLU:HG3	1.99	0.45
1:B:408:ASP:HB2	1:B:531:GLY:CA	2.47	0.45
1:B:61:LEU:HD22	1:B:307:ILE:HD12	1.99	0.45
1:B:791:GLN:HE22	1:B:897:MET:HB3	1.82	0.45
1:B:82:GLU:H	1:B:82:GLU:CD	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:C	1:A:27:ASP:N	2.70	0.44
1:A:369:ILE:HD13	1:A:379:LEU:HD22	1.98	0.44
1:A:419:LEU:HD11	1:A:479:MET:HB2	1.98	0.44
1:B:419:LEU:HD11	1:B:479:MET:HB2	1.98	0.44
1:A:168:ILE:HA	1:A:219:ALA:HB2	1.99	0.44
1:A:447:THR:O	1:A:451:LYS:HG3	2.17	0.44
1:B:428:ASN:HB2	1:B:435:GLU:HG3	1.99	0.44
1:B:974:SER:C	1:B:976:PRO:HD2	2.38	0.44
1:A:421:ASN:HD21	1:A:442:GLU:HB3	1.82	0.44
1:A:499:SER:CB	1:A:500:PRO:HD2	2.44	0.44
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.53	0.44
1:A:475:ILE:HA	1:A:478:LEU:HD13	1.99	0.44
1:A:690:TYR:C	1:A:692:GLN:H	2.21	0.44
1:A:691:LEU:O	1:A:696:GLU:HB2	2.17	0.44
1:B:628:ASN:HD21	1:B:631:THR:HB	1.83	0.44
1:B:690:TYR:C	1:B:692:GLN:N	2.69	0.44
1:B:671:ARG:HD2	1:B:694:TYR:CE1	2.53	0.44
1:B:833:LEU:CG	1:B:837:TYR:HE2	2.30	0.44
1:A:61:LEU:HD21	1:A:257:GLY:HA2	1.99	0.44
1:A:82:GLU:CD	1:A:82:GLU:H	2.20	0.44
1:A:981:ASP:O	1:A:984:LEU:N	2.51	0.44
1:B:667:ARG:HB2	1:B:690:TYR:CE1	2.53	0.44
1:B:355:THR:OG1	1:B:720:MET:HE2	2.17	0.44
1:A:134:ARG:HB3	1:A:135:LYS:H	1.72	0.44
1:B:416:ILE:O	1:B:417:CYS:C	2.56	0.44
1:B:926:PRO:HA	1:B:927:PRO:HD3	1.93	0.44
1:A:332:ILE:O	1:A:733:MET:HA	2.18	0.44
1:A:516:GLY:O	1:A:563:ALA:N	2.49	0.44
1:A:791:GLN:O	1:A:792:LEU:C	2.55	0.44
1:A:865:VAL:O	1:A:868:HIS:CB	2.66	0.44
1:A:895:GLU:N	1:A:896:PRO:CD	2.78	0.44
1:A:974:SER:C	1:A:976:PRO:HD2	2.38	0.44
1:B:179:ILE:HD13	1:B:211:GLY:O	2.17	0.44
1:B:246:LYS:HB3	1:B:250:GLN:HE21	1.82	0.44
1:B:670:CYS:O	1:B:691:LEU:HD11	2.18	0.44
1:B:865:VAL:O	1:B:868:HIS:CB	2.66	0.44
1:A:260:LEU:CD1	2:A:1001:TG1:H252	2.47	0.44
1:A:52:LEU:HD11	1:A:109:GLU:HG3	1.99	0.44
1:A:650:ASP:OD2	1:A:651:ARG:HG2	2.18	0.44
1:A:833:LEU:CG	1:A:837:TYR:HE2	2.30	0.44
1:B:6:SER:OG	1:B:197:PRO:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:LYS:HB2	1:A:654:THR:CG2	2.48	0.43
1:B:260:LEU:CD1	2:B:1002:TG1:H252	2.47	0.43
1:B:368:ILE:HD11	1:B:410:LEU:HG	2.00	0.43
1:B:524:ARG:HB2	1:B:591:LEU:HD12	2.00	0.43
1:B:551:GLU:O	1:B:555:GLY:N	2.44	0.43
1:B:777:LEU:O	1:B:778:THR:C	2.56	0.43
1:A:165:ILE:HD11	1:A:208:LEU:HD21	2.00	0.43
1:A:6:SER:OG	1:A:197:PRO:HA	2.18	0.43
1:A:408:ASP:HB2	1:A:531:GLY:CA	2.47	0.43
1:B:421:ASN:HD21	1:B:442:GLU:HB3	1.82	0.43
1:A:122:TYR:HE1	1:A:726:VAL:HG13	1.83	0.43
1:A:758:LYS:HG3	1:A:828:LEU:CD2	2.41	0.43
1:B:165:ILE:HD11	1:B:208:LEU:HD21	2.00	0.43
1:B:873:PHE:HD1	1:B:875:GLN:N	2.12	0.43
1:A:235:ILE:HD13	1:A:705:VAL:O	2.19	0.43
1:A:61:LEU:HD22	1:A:307:ILE:HD12	1.99	0.43
1:B:168:ILE:HA	1:B:219:ALA:HB2	1.99	0.43
1:B:342:LEU:CD1	1:B:716:ILE:HD13	2.48	0.43
1:B:791:GLN:HG3	1:B:791:GLN:H	1.61	0.43
1:B:915:SER:O	1:B:917:SER:N	2.51	0.43
1:A:382:PHE:HD2	1:A:395:VAL:HG12	1.83	0.43
1:A:743:ILE:O	1:A:747:VAL:HG23	2.19	0.43
1:B:38:HIS:CE1	1:B:143:ARG:HH12	2.37	0.43
1:B:61:LEU:HD21	1:B:257:GLY:HA2	1.99	0.43
1:B:369:ILE:HD13	1:B:379:LEU:HD22	1.98	0.43
1:B:691:LEU:O	1:B:696:GLU:HB2	2.17	0.43
1:A:247:THR:HG22	1:A:250:GLN:N	2.13	0.43
1:A:38:HIS:CD2	1:A:143:ARG:NH2	2.87	0.43
1:A:368:ILE:HD11	1:A:410:LEU:HG	2.00	0.43
1:A:596:VAL:CG1	1:A:597:VAL:N	2.82	0.43
1:A:628:ASN:HD21	1:A:631:THR:HB	1.83	0.43
1:A:670:CYS:O	1:A:691:LEU:HD11	2.18	0.43
1:A:667:ARG:HB2	1:A:690:TYR:CE1	2.53	0.43
1:B:928:TRP:HA	1:B:934:LEU:HD12	2.00	0.43
1:B:93:VAL:O	1:B:94:ILE:C	2.57	0.43
1:B:981:ASP:O	1:B:984:LEU:N	2.51	0.43
1:A:510:ASN:HD22	1:A:510:ASN:HA	1.67	0.43
1:A:915:SER:O	1:A:917:SER:N	2.51	0.43
1:A:913:LEU:HD21	1:A:937:ILE:CD1	2.49	0.43
1:B:2:GLU:O	1:B:2:GLU:HG2	2.18	0.43
1:B:1:MET:N	1:B:36:TYR:CZ	2.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:ALA:HA	1:B:809:PHE:CD2	2.54	0.43
1:A:338:SER:O	1:A:340:GLU:N	2.52	0.43
1:A:486:GLU:H	1:A:486:GLU:HG3	1.55	0.43
1:A:948:LEU:O	1:A:954:PRO:HB3	2.19	0.43
1:B:380:ASN:O	1:B:382:PHE:CD1	2.72	0.43
1:B:915:SER:C	1:B:917:SER:N	2.72	0.43
1:B:263:VAL:O	1:B:266:LEU:N	2.50	0.43
1:B:332:ILE:O	1:B:733:MET:HA	2.18	0.43
1:B:519:GLU:O	1:B:523:ASP:HB2	2.19	0.43
1:B:690:TYR:C	1:B:692:GLN:H	2.21	0.43
1:B:6:SER:HA	1:B:194:VAL:O	2.19	0.43
1:A:519:GLU:O	1:A:523:ASP:HB2	2.19	0.42
1:A:524:ARG:HB2	1:A:591:LEU:HD12	2.01	0.42
1:A:547:SER:O	1:A:550:LYS:N	2.52	0.42
1:A:58:GLU:HG2	1:A:63:ARG:NH2	2.34	0.42
1:A:777:LEU:C	1:A:779:ALA:N	2.72	0.42
1:A:925:MET:HE3	1:A:985:LYS:HZ3	1.84	0.42
1:B:122:TYR:HE1	1:B:726:VAL:HG13	1.83	0.42
1:B:959:LEU:HG	1:B:960:LYS:H	1.84	0.42
1:A:1:MET:N	1:A:36:TYR:CZ	2.83	0.42
1:A:757:MET:HA	1:A:760:PHE:CD2	2.54	0.42
1:B:38:HIS:CD2	1:B:143:ARG:NH2	2.86	0.42
1:B:39:ASN:CB	1:B:226:THR:HB	2.50	0.42
1:B:450:GLU:OE2	1:B:467:ARG:O	2.37	0.42
1:B:562:LEU:HA	1:B:562:LEU:HD12	1.88	0.42
1:B:58:GLU:HG2	1:B:63:ARG:NH2	2.34	0.42
1:B:948:LEU:O	1:B:954:PRO:HB3	2.19	0.42
1:A:170:SER:HB3	1:A:218:LYS:H	1.84	0.42
1:A:206:ASN:OD1	1:A:206:ASN:C	2.58	0.42
1:A:2:GLU:HG2	1:A:2:GLU:O	2.18	0.42
1:A:370:ASP:HB3	1:A:378:SER:HG	1.83	0.42
1:A:953:LEU:C	1:A:955:MET:H	2.23	0.42
1:A:977:VAL:CG1	1:A:978:ILE:N	2.83	0.42
1:B:165:ILE:HD11	1:B:208:LEU:CD2	2.49	0.42
1:B:382:PHE:HD2	1:B:395:VAL:HG12	1.83	0.42
1:B:547:SER:O	1:B:550:LYS:N	2.52	0.42
1:B:650:ASP:OD2	1:B:651:ARG:HG2	2.18	0.42
1:B:691:LEU:HA	1:B:691:LEU:HD12	1.79	0.42
1:B:705:VAL:HG23	1:B:706:ASN:N	2.35	0.42
1:A:165:ILE:HD11	1:A:208:LEU:CD2	2.49	0.42
1:A:256:PHE:HE2	1:A:308:PRO:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:GLU:HA	1:B:660:ASP:OD2	2.20	0.42
1:B:687:ILE:HG22	1:B:691:LEU:HD22	2.00	0.42
1:A:6:SER:HA	1:A:194:VAL:O	2.19	0.42
1:A:312:PRO:HA	1:A:315:ILE:CG1	2.50	0.42
1:A:38:HIS:CE1	1:A:143:ARG:HH12	2.37	0.42
1:A:483:PHE:CE2	1:A:485:LEU:HD21	2.48	0.42
1:A:535:VAL:CB	1:A:536:PRO:HD2	2.47	0.42
1:A:900:ALA:O	1:A:903:VAL:HB	2.20	0.42
1:A:959:LEU:HG	1:A:960:LYS:H	1.84	0.42
1:B:894:PRO:HA	1:B:897:MET:HE3	2.02	0.42
1:B:900:ALA:O	1:B:903:VAL:HB	2.20	0.42
1:A:380:ASN:O	1:A:382:PHE:CD1	2.72	0.42
1:A:450:GLU:OE2	1:A:467:ARG:O	2.37	0.42
1:A:547:SER:O	1:A:550:LYS:HB3	2.20	0.42
1:A:735:LEU:HB3	1:A:742:THR:HG21	2.02	0.42
1:A:806:ALA:HA	1:A:809:PHE:CD2	2.54	0.42
1:B:235:ILE:HD13	1:B:705:VAL:O	2.19	0.42
1:B:256:PHE:HE2	1:B:308:PRO:HG3	1.84	0.42
1:B:312:PRO:HA	1:B:315:ILE:CG1	2.50	0.42
1:B:544:LYS:O	1:B:544:LYS:HD3	2.19	0.42
1:B:653:TYR:CZ	1:B:669:ALA:HB1	2.55	0.42
1:B:743:ILE:O	1:B:747:VAL:HG23	2.19	0.42
1:A:39:ASN:CB	1:A:226:THR:HB	2.50	0.42
1:A:519:GLU:HG2	1:A:520:GLY:H	1.84	0.42
1:A:915:SER:C	1:A:917:SER:N	2.72	0.42
1:A:928:TRP:HA	1:A:934:LEU:HD12	2.00	0.42
1:B:385:THR:O	1:B:393:GLY:HA3	2.20	0.42
1:B:596:VAL:CG1	1:B:597:VAL:N	2.82	0.42
1:B:966:GLN:HA	1:B:966:GLN:HE21	1.85	0.42
1:A:159:VAL:CG1	1:A:163:ILE:HD12	2.50	0.42
1:A:572:LYS:O	1:A:575:GLU:HB2	2.20	0.42
1:A:653:TYR:CZ	1:A:669:ALA:HB1	2.55	0.42
1:A:705:VAL:HG23	1:A:706:ASN:N	2.35	0.42
1:A:777:LEU:O	1:A:778:THR:C	2.56	0.42
1:A:865:VAL:O	1:A:868:HIS:HB2	2.19	0.42
1:A:981:ASP:HB3	1:A:982:GLU:H	1.72	0.42
1:B:324:ARG:C	1:B:324:ARG:CD	2.85	0.42
1:B:735:LEU:HB3	1:B:742:THR:HG21	2.02	0.42
1:B:802:LEU:HD22	1:B:802:LEU:N	2.35	0.42
1:B:913:LEU:HD21	1:B:937:ILE:CD1	2.49	0.42
1:B:925:MET:HE3	1:B:985:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:HIS:CA	1:A:282:PRO:HD2	2.45	0.42
1:A:657:GLU:HA	1:A:660:ASP:OD2	2.20	0.42
1:A:93:VAL:O	1:A:94:ILE:C	2.57	0.42
1:B:170:SER:HB3	1:B:218:LYS:H	1.84	0.42
1:B:338:SER:C	1:B:340:GLU:H	2.23	0.42
1:B:382:PHE:CD2	1:B:395:VAL:HG12	2.55	0.42
1:B:629:LYS:HB2	1:B:654:THR:CG2	2.48	0.42
1:A:488:SER:C	1:A:490:ASP:N	2.74	0.42
1:A:593:PHE:CZ	1:A:596:VAL:HG23	2.54	0.42
1:A:737:ASP:C	1:A:739:ASN:N	2.73	0.42
1:A:802:LEU:N	1:A:802:LEU:HD22	2.35	0.42
1:A:966:GLN:HA	1:A:966:GLN:HE21	1.85	0.42
1:B:593:PHE:CE1	1:B:595:GLY:N	2.88	0.42
1:A:59:ASP:OD2	1:A:61:LEU:HB2	2.20	0.41
1:A:687:ILE:HG22	1:A:691:LEU:HD22	2.00	0.41
1:A:544:LYS:HD3	1:A:544:LYS:O	2.19	0.41
1:B:206:ASN:C	1:B:206:ASN:OD1	2.58	0.41
1:B:321:LEU:O	1:B:324:ARG:HG3	2.21	0.41
1:B:757:MET:HA	1:B:760:PHE:CD2	2.54	0.41
1:B:865:VAL:O	1:B:868:HIS:HB2	2.20	0.41
1:B:977:VAL:CG1	1:B:978:ILE:N	2.83	0.41
1:A:130:TYR:HB2	1:A:150:ILE:CG1	2.44	0.41
1:A:385:THR:O	1:A:393:GLY:HA3	2.20	0.41
1:A:368:ILE:CD1	1:A:410:LEU:CD2	2.96	0.41
1:A:496:VAL:HG12	1:A:513:PHE:HB2	2.02	0.41
1:A:580:ASP:O	1:A:583:ARG:N	2.45	0.41
1:A:894:PRO:HA	1:A:897:MET:HE3	2.02	0.41
1:B:496:VAL:HG12	1:B:513:PHE:HB2	2.02	0.41
1:B:59:ASP:OD2	1:B:61:LEU:HB2	2.20	0.41
1:A:388:THR:OG1	1:A:389:TYR:N	2.53	0.41
1:A:382:PHE:CD2	1:A:395:VAL:HG12	2.55	0.41
1:A:628:ASN:ND2	1:A:631:THR:HB	2.35	0.41
1:B:71:ILE:HG23	1:B:296:PHE:HD2	1.85	0.41
1:B:338:SER:O	1:B:340:GLU:N	2.52	0.41
1:B:371:LYS:HE3	1:B:371:LYS:HB2	1.97	0.41
1:B:519:GLU:HG2	1:B:520:GLY:H	1.84	0.41
1:B:880:HIS:N	1:B:881:PRO:CD	2.83	0.41
1:B:336:LEU:HB2	1:B:337:PRO:HD3	2.03	0.41
1:B:499:SER:HB2	1:B:500:PRO:CD	2.48	0.41
1:A:236:ARG:NH1	1:A:237:ASP:OD2	2.50	0.41
1:A:338:SER:C	1:A:340:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:ARG:HB3	1:A:607:VAL:CG1	2.40	0.41
1:B:159:VAL:CG1	1:B:163:ILE:HD12	2.50	0.41
1:B:547:SER:O	1:B:550:LYS:HB3	2.20	0.41
1:B:662:PRO:O	1:B:664:ALA:N	2.54	0.41
1:B:981:ASP:OD2	1:B:985:LYS:HD2	2.21	0.41
1:A:349:CYS:HA	1:A:622:ILE:O	2.21	0.41
1:A:593:PHE:CE1	1:A:595:GLY:N	2.88	0.41
1:A:662:PRO:O	1:A:664:ALA:N	2.54	0.41
1:B:174:ARG:HA	1:B:187:VAL:O	2.21	0.41
1:B:396:LEU:HA	1:B:402:ILE:HD12	2.03	0.41
1:B:419:LEU:CD1	1:B:513:PHE:HE2	2.34	0.41
1:B:678:ARG:HH11	1:B:678:ARG:HG3	1.86	0.41
1:B:754:TYR:HA	1:B:757:MET:HE2	2.03	0.41
1:B:764:LEU:HD12	1:B:764:LEU:HA	1.75	0.41
1:B:953:LEU:C	1:B:955:MET:H	2.23	0.41
1:B:840:ILE:HD13	1:B:980:LEU:CD2	2.51	0.41
1:A:222:ILE:HG23	1:A:222:ILE:O	2.21	0.41
1:A:873:PHE:CB	1:A:875:GLN:HE21	2.34	0.41
1:B:222:ILE:HG23	1:B:222:ILE:O	2.21	0.41
1:A:227:GLY:C	1:A:229:SER:H	2.24	0.41
1:A:453:ASN:CG	1:A:471:CYS:SG	2.99	0.41
1:A:342:LEU:CD1	1:A:716:ILE:HD13	2.48	0.41
1:A:816:ILE:HG23	1:A:817:MET:HG2	2.03	0.41
1:B:400:LYS:HA	1:B:401:PRO:HD2	1.93	0.41
1:B:511:LYS:HA	1:B:511:LYS:HD3	1.97	0.41
1:B:593:PHE:CZ	1:B:596:VAL:HG23	2.55	0.41
1:B:628:ASN:ND2	1:B:631:THR:HB	2.35	0.41
1:B:65:LEU:O	1:B:69:ALA:N	2.54	0.41
1:B:867:TYR:CD1	1:B:867:TYR:N	2.89	0.41
1:A:71:ILE:HG23	1:A:296:PHE:HD2	1.85	0.41
1:A:759:GLN:O	1:A:762:ARG:N	2.54	0.41
1:A:867:TYR:CD1	1:A:867:TYR:N	2.89	0.41
1:A:950:VAL:O	1:A:952:PRO:CD	2.69	0.41
1:B:380:ASN:O	1:B:382:PHE:HD1	2.04	0.41
1:B:737:ASP:C	1:B:739:ASN:N	2.73	0.41
1:B:777:LEU:C	1:B:779:ALA:N	2.72	0.41
1:B:912:ALA:O	1:B:933:LEU:HD21	2.21	0.41
1:A:178:SER:O	1:A:179:ILE:C	2.59	0.41
1:A:480:LYS:O	1:A:498:CYS:HB2	2.21	0.41
1:A:562:LEU:HA	1:A:562:LEU:HD12	1.88	0.41
1:B:154:ALA:HB2	1:B:218:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ASN:CG	1:B:471:CYS:SG	2.99	0.41
1:B:453:ASN:ND2	1:B:471:CYS:SG	2.94	0.41
1:B:349:CYS:HA	1:B:622:ILE:O	2.21	0.41
1:B:950:VAL:O	1:B:952:PRO:CD	2.69	0.41
1:A:154:ALA:HB2	1:A:218:LYS:HG3	2.03	0.40
1:A:281:ASP:O	1:A:282:PRO:C	2.60	0.40
1:A:678:ARG:HH11	1:A:678:ARG:HG3	1.86	0.40
1:A:758:LYS:HZ1	1:A:822:ARG:HE	1.69	0.40
1:A:91:PRO:HG2	1:A:92:PHE:H	1.86	0.40
1:B:246:LYS:O	1:B:247:THR:C	2.60	0.40
1:B:873:PHE:CB	1:B:875:GLN:HE21	2.34	0.40
1:A:174:ARG:HA	1:A:187:VAL:O	2.21	0.40
1:A:453:ASN:ND2	1:A:471:CYS:SG	2.94	0.40
1:A:788:ILE:CG2	1:A:789:PRO:HD2	2.38	0.40
1:A:981:ASP:OD2	1:A:985:LYS:HD2	2.21	0.40
1:B:281:ASP:O	1:B:282:PRO:C	2.60	0.40
1:B:513:PHE:CD1	1:B:566:THR:HG22	2.56	0.40
1:B:572:LYS:O	1:B:575:GLU:HB2	2.20	0.40
1:B:962:LEU:C	1:B:964:LEU:N	2.75	0.40
1:A:60:LEU:O	1:A:64:ILE:HG12	2.22	0.40
1:B:178:SER:O	1:B:179:ILE:C	2.59	0.40
1:B:368:ILE:CD1	1:B:410:LEU:CD2	2.96	0.40
1:B:546:LEU:O	1:B:547:SER:C	2.59	0.40
1:A:350:SER:HA	1:A:701:THR:HG22	2.01	0.40
1:A:428:ASN:HB2	1:A:435:GLU:HG2	2.03	0.40
1:A:459:VAL:C	1:A:461:ASN:H	2.24	0.40
1:A:622:ILE:CD1	1:A:691:LEU:HD21	2.52	0.40
1:A:65:LEU:O	1:A:69:ALA:N	2.54	0.40
1:A:350:SER:CA	1:A:701:THR:HG21	2.48	0.40
1:A:737:ASP:C	1:A:739:ASN:H	2.25	0.40
1:B:737:ASP:C	1:B:739:ASN:H	2.25	0.40
1:B:737:ASP:O	1:B:739:ASN:N	2.55	0.40
1:A:352:LYS:HA	1:A:356:LEU:HB2	2.04	0.40
1:A:499:SER:HB2	1:A:500:PRO:CD	2.48	0.40
1:A:764:LEU:HA	1:A:764:LEU:HD12	1.75	0.40
1:A:802:LEU:H	1:A:802:LEU:HD22	1.85	0.40
1:A:840:ILE:HD13	1:A:980:LEU:CD2	2.51	0.40
1:B:250:GLN:O	1:B:254:ASP:OD2	2.40	0.40
1:B:25:THR:O	1:B:26:PRO:C	2.60	0.40
1:B:273:LEU:HA	1:B:276:ILE:HD11	2.03	0.40
1:B:480:LYS:O	1:B:498:CYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:ILE:HG13	1:B:635:ILE:H	1.70	0.40
1:B:60:LEU:O	1:B:64:ILE:HG12	2.22	0.40
1:B:698:THR:CG2	1:B:699:ALA:N	2.85	0.40
1:B:857:MET:O	1:B:859:ALA:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	992/994 (100%)	760 (77%)	185 (19%)	47 (5%)	2	14
1	B	992/994 (100%)	760 (77%)	185 (19%)	47 (5%)	2	14
All	All	1984/1988 (100%)	1520 (77%)	370 (19%)	94 (5%)	2	14

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	782	GLY
1	A	864	GLY
1	A	951	ASP
1	A	965	THR
1	B	782	GLY
1	B	864	GLY
1	B	951	ASP
1	B	965	THR
1	A	94	ILE
1	A	374	GLY
1	A	581	SER
1	A	857	MET
1	A	858	TYR
1	A	883	PHE

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Mol	Chain	Res	Type
1	A	964	LEU
1	A	981	ASP
1	B	94	ILE
1	B	374	GLY
1	B	581	SER
1	B	857	MET
1	B	858	TYR
1	B	883	PHE
1	B	964	LEU
1	B	981	ASP
1	A	280	ASN
1	A	281	ASP
1	A	454	VAL
1	A	467	ARG
1	A	470	ALA
1	A	500	PRO
1	A	519	GLU
1	A	521	VAL
1	A	536	PRO
1	A	540	PRO
1	A	644	GLU
1	A	663	LEU
1	A	795	VAL
1	B	280	ASN
1	B	281	ASP
1	B	454	VAL
1	B	467	ARG
1	B	470	ALA
1	B	500	PRO
1	B	519	GLU
1	B	521	VAL
1	B	536	PRO
1	B	540	PRO
1	B	644	GLU
1	B	663	LEU
1	B	795	VAL
1	A	286	GLY
1	A	507	ALA
1	A	735	LEU
1	A	758	LYS
1	A	916	LEU
1	A	982	GLU

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Mol	Chain	Res	Type
1	B	286	GLY
1	B	507	ALA
1	B	735	LEU
1	B	758	LYS
1	B	916	LEU
1	B	982	GLU
1	A	283	VAL
1	A	352	LYS
1	A	578	LEU
1	A	681	PRO
1	A	869	GLN
1	B	283	VAL
1	B	352	LYS
1	B	578	LEU
1	B	681	PRO
1	B	869	GLN
1	A	669	ALA
1	A	716	ILE
1	A	975	LEU
1	B	669	ALA
1	B	716	ILE
1	B	975	LEU
1	A	17	GLY
1	A	228	VAL
1	A	386	GLY
1	A	952	PRO
1	B	17	GLY
1	B	228	VAL
1	B	386	GLY
1	B	952	PRO
1	A	865	VAL
1	A	950	VAL
1	B	865	VAL
1	B	950	VAL
1	A	185	VAL
1	B	185	VAL
1	A	195	PRO
1	B	195	PRO

### 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	840/840 (100%)	766 (91%)	74 (9%)	10	36
1	B	840/840 (100%)	766 (91%)	74 (9%)	10	36
All	All	1680/1680 (100%)	1532 (91%)	148 (9%)	10	36

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	35	LYS
1	A	44	GLU
1	A	45	GLU
1	A	78	PHE
1	A	83	GLU
1	A	96	LEU
1	A	113	GLU
1	A	153	VAL
1	A	155	VAL
1	A	160	PRO
1	A	175	VAL
1	A	200	VAL
1	A	205	LYS
1	A	218	LYS
1	A	220	LEU
1	A	236	ARG
1	A	245	ASP
1	A	247	THR
1	A	302	LEU
1	A	365	LYS
1	A	371	LYS
1	A	373	ASP
1	A	381	GLU
1	A	384	ILE
1	A	402	ILE
1	A	411	VAL

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Mol	Chain	Res	Type
1	A	422	ASP
1	A	429	GLU
1	A	431	LYS
1	A	449	VAL
1	A	450	GLU
1	A	484	THR
1	A	486	GLU
1	A	491	ARG
1	A	510	ASN
1	A	512	MET
1	A	518	PRO
1	A	519	GLU
1	A	523	ASP
1	A	538	THR
1	A	544	LYS
1	A	554	THR
1	A	574	GLU
1	A	597	VAL
1	A	605	LYS
1	A	612	GLN
1	A	621	VAL
1	A	628	ASN
1	A	642	PHE
1	A	656	ARG
1	A	691	LEU
1	A	692	GLN
1	A	707	ASP
1	A	726	VAL
1	A	732	GLU
1	A	739	ASN
1	A	760	PHE
1	A	764	LEU
1	A	766	SER
1	A	788	ILE
1	A	793	LEU
1	A	796	ASN
1	A	814	LEU
1	A	815	ASP
1	A	816	ILE
1	A	818	ASP
1	A	883	PHE
1	A	956	ILE

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Mol	Chain	Res	Type
1	A	958	LYS
1	A	972	LYS
1	A	973	ILE
1	A	982	GLU
1	A	986	PHE
1	B	34	GLU
1	B	35	LYS
1	B	44	GLU
1	B	45	GLU
1	B	78	PHE
1	B	83	GLU
1	B	96	LEU
1	B	113	GLU
1	B	153	VAL
1	B	155	VAL
1	B	160	PRO
1	B	175	VAL
1	B	200	VAL
1	B	205	LYS
1	B	218	LYS
1	B	220	LEU
1	B	236	ARG
1	B	245	ASP
1	B	247	THR
1	B	302	LEU
1	B	365	LYS
1	B	371	LYS
1	B	373	ASP
1	B	381	GLU
1	B	384	ILE
1	B	402	ILE
1	B	411	VAL
1	B	422	ASP
1	B	429	GLU
1	B	431	LYS
1	B	449	VAL
1	B	450	GLU
1	B	484	THR
1	B	486	GLU
1	B	491	ARG
1	B	510	ASN
1	B	512	MET

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Mol	Chain	Res	Type
1	B	518	PRO
1	B	519	GLU
1	B	523	ASP
1	B	538	THR
1	B	544	LYS
1	B	554	THR
1	B	574	GLU
1	B	597	VAL
1	B	605	LYS
1	B	612	GLN
1	B	621	VAL
1	B	628	ASN
1	B	642	PHE
1	B	656	ARG
1	B	691	LEU
1	B	692	GLN
1	B	707	ASP
1	B	726	VAL
1	B	732	GLU
1	B	739	ASN
1	B	760	PHE
1	B	764	LEU
1	B	766	SER
1	B	788	ILE
1	B	793	LEU
1	B	796	ASN
1	B	814	LEU
1	B	815	ASP
1	B	816	ILE
1	B	818	ASP
1	B	883	PHE
1	B	956	ILE
1	B	958	LYS
1	B	972	LYS
1	B	973	ILE
1	B	982	GLU
1	B	986	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS

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Mol	Chain	Res	Type
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	380	ASN
1	A	461	ASN
1	A	510	ASN
1	A	628	ASN
1	A	739	ASN
1	A	768	ASN
1	A	872	HIS
1	A	875	GLN
1	A	914	ASN
1	A	919	ASN
1	A	966	GLN
1	B	38	HIS
1	B	250	GLN
1	B	275	ASN
1	B	359	ASN
1	B	380	ASN
1	B	461	ASN
1	B	510	ASN
1	B	628	ASN
1	B	739	ASN
1	B	768	ASN
1	B	872	HIS
1	B	875	GLN
1	B	914	ASN
1	B	919	ASN
1	B	966	GLN

### 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 carbohydrates 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	$\# Z  > 2$
2	TG1	A	1001	-	43,48,48	1.82	15 (34%)	44,72,72	1.96	9 (20%)
2	TG1	B	1002	-	43,48,48	1.82	14 (32%)	44,72,72	1.97	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TG1	A	1001	-	-	9/33/99/99	0/3/3/3
2	TG1	B	1002	-	-	9/33/99/99	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	TG1	O4-C21	5.60	1.33	1.21
2	A	1001	TG1	O4-C21	5.57	1.33	1.21
2	A	1001	TG1	O3-C3	3.35	1.51	1.44
2	B	1002	TG1	O3-C3	3.35	1.51	1.44
2	A	1001	TG1	O1-C13	3.23	1.43	1.34
2	B	1002	TG1	O1-C13	3.23	1.43	1.34
2	A	1001	TG1	O6-C7	3.14	1.48	1.43
2	B	1002	TG1	O6-C7	3.14	1.48	1.43
2	A	1001	TG1	C34-C11	3.13	1.57	1.53
2	B	1002	TG1	C34-C11	3.13	1.57	1.53
2	A	1001	TG1	C11-C7	3.02	1.59	1.55
2	B	1002	TG1	C11-C7	3.02	1.59	1.55
2	A	1001	TG1	O7-C27	2.81	1.42	1.34
2	B	1002	TG1	O7-C27	2.81	1.42	1.34
2	A	1001	TG1	C9-C10	2.52	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	TG1	C9-C10	2.52	1.58	1.54
2	A	1001	TG1	C4-C5	2.50	1.36	1.34
2	B	1002	TG1	C4-C5	2.50	1.36	1.34
2	A	1001	TG1	C21-C22	2.41	1.58	1.50
2	B	1002	TG1	C21-C22	2.41	1.58	1.50
2	A	1001	TG1	C31-C10	2.27	1.57	1.52
2	B	1002	TG1	C31-C10	2.27	1.57	1.52
2	B	1002	TG1	C1-C2	2.23	1.58	1.54
2	A	1001	TG1	C1-C2	2.22	1.58	1.54
2	A	1001	TG1	O11-C11	2.12	1.46	1.42
2	B	1002	TG1	O11-C11	2.12	1.46	1.42
2	B	1002	TG1	C9-C8	2.04	1.55	1.52
2	A	1001	TG1	C9-C8	2.04	1.55	1.52
2	A	1001	TG1	C3-C4	2.01	1.53	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	TG1	C10-O9-C32	5.62	134.87	121.53
2	B	1002	TG1	C10-O9-C32	5.62	134.87	121.53
2	B	1002	TG1	O12-C12-C11	-4.21	124.05	128.28
2	A	1001	TG1	O12-C12-C11	-4.18	124.08	128.28
2	B	1002	TG1	O7-C8-C9	4.09	113.95	106.63
2	A	1001	TG1	O7-C8-C9	4.08	113.92	106.63
2	A	1001	TG1	C7-C6-C5	3.93	125.46	115.41
2	B	1002	TG1	C7-C6-C5	3.93	125.46	115.41
2	A	1001	TG1	C11-C7-C6	-3.39	96.50	103.03
2	B	1002	TG1	C11-C7-C6	-3.39	96.50	103.03
2	B	1002	TG1	O5-C12-O12	3.31	126.01	121.62
2	A	1001	TG1	O5-C12-O12	3.31	126.00	121.62
2	A	1001	TG1	C24-C22-C21	3.02	132.74	120.78
2	B	1002	TG1	C24-C22-C21	3.02	132.74	120.78
2	A	1001	TG1	C23-C22-C21	-2.72	109.29	116.09
2	B	1002	TG1	C23-C22-C21	-2.72	109.29	116.09
2	A	1001	TG1	C2-O1-C13	-2.39	113.54	117.53
2	B	1002	TG1	C2-O1-C13	-2.39	113.54	117.53

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	TG1	O3-C21-C22-C23

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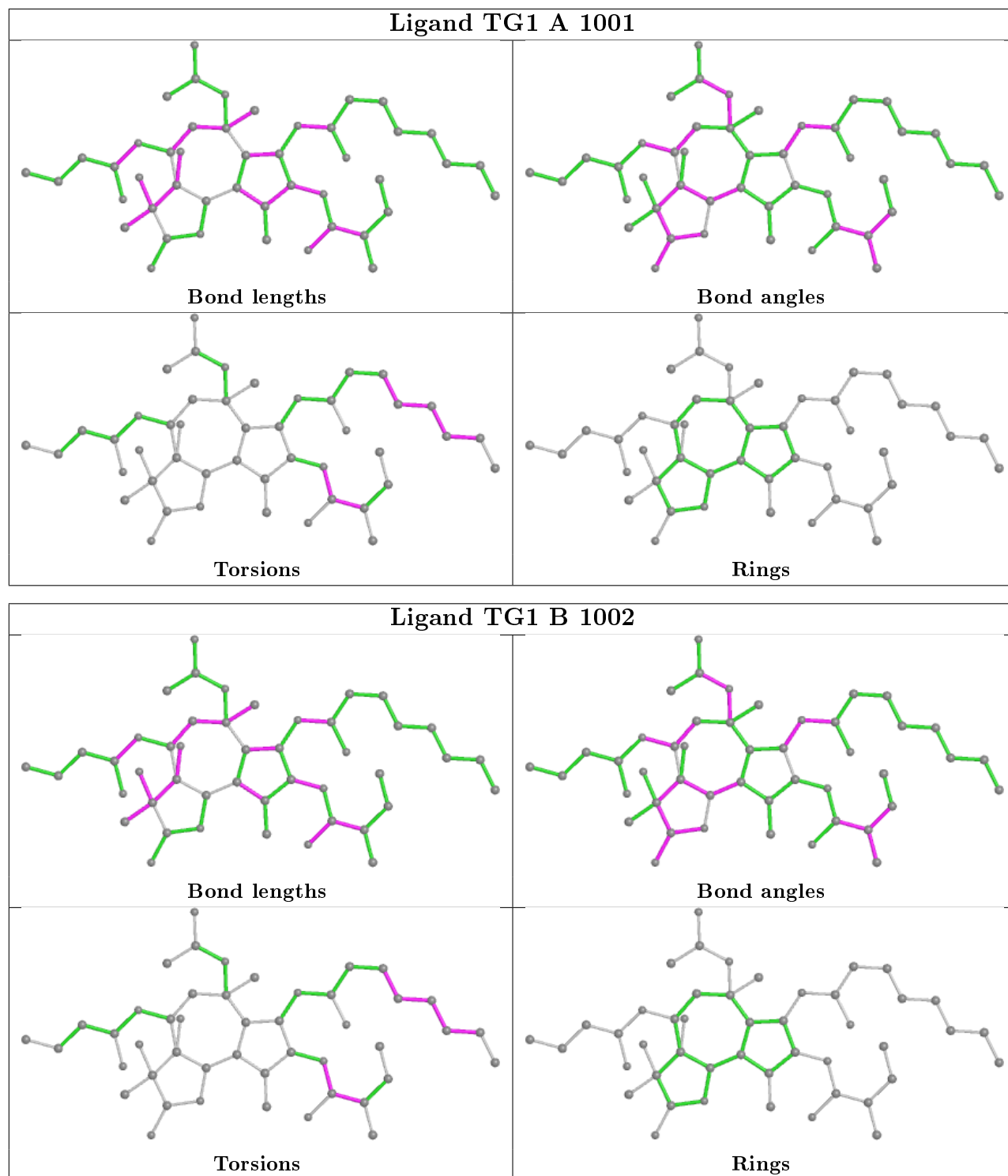
Mol	Chain	Res	Type	Atoms
2	A	1001	TG1	O3-C21-C22-C24
2	A	1001	TG1	O4-C21-C22-C23
2	B	1002	TG1	O3-C21-C22-C23
2	B	1002	TG1	O3-C21-C22-C24
2	B	1002	TG1	O4-C21-C22-C23
2	A	1001	TG1	O4-C21-C22-C24
2	B	1002	TG1	O4-C21-C22-C24
2	A	1001	TG1	C22-C21-O3-C3
2	B	1002	TG1	C22-C21-O3-C3
2	A	1001	TG1	C15-C16-C17-C18
2	B	1002	TG1	C15-C16-C17-C18
2	A	1001	TG1	C16-C17-C18-C19
2	B	1002	TG1	C16-C17-C18-C19
2	A	1001	TG1	C14-C15-C16-C17
2	B	1002	TG1	C14-C15-C16-C17
2	A	1001	TG1	C17-C18-C19-C20
2	B	1002	TG1	C17-C18-C19-C20

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	TG1	5	0
2	B	1002	TG1	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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.