



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:02 PM UTC

PDB ID : 3RFU / pdb_00003rfu
Title : Crystal structure of a copper-transporting PIB-type ATPase
Authors : Gourdon, P.; Liu, X.; Skjorringe, T.; Morth, J.P.; Birk Moller, L.; Panyella Pedersen, B.; Nissen, P.
Deposited on : 2011-04-07
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

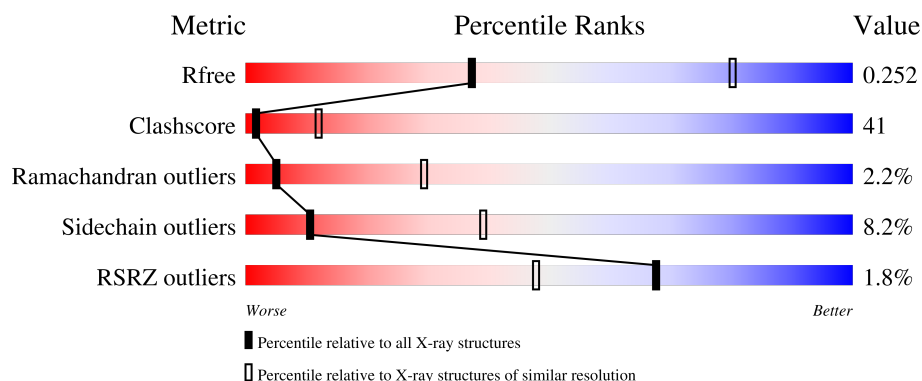
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	736	% 36% 47% 7% 10%
1	B	736	2% 37% 47% 7% 10%
1	C	736	2% 36% 47% 7% 10%
1	D	736	% 37% 47% 7% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ALF	A	995	-	-	X	-

2 Entry composition [i](#)

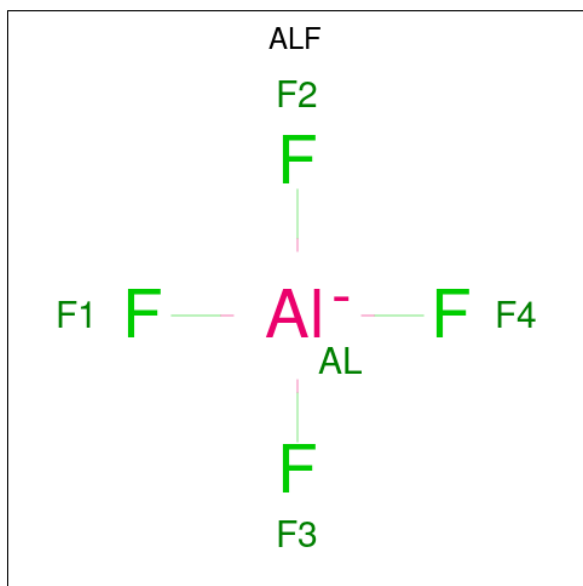
There are 4 unique types of molecules in this entry. The entry contains 19764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Copper efflux ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			
1	B	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			
1	C	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			
1	D	663	Total	C	N	O	S	0	0	0
			4934	3156	844	909	25			

- Molecule 2 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Al	F	0	0
			5	1	4		
2	B	1	Total	Al	F	0	0
			5	1	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	Al	F	0	0
			5	1	4		
2	D	1	Total	Al	F	0	0
			5	1	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

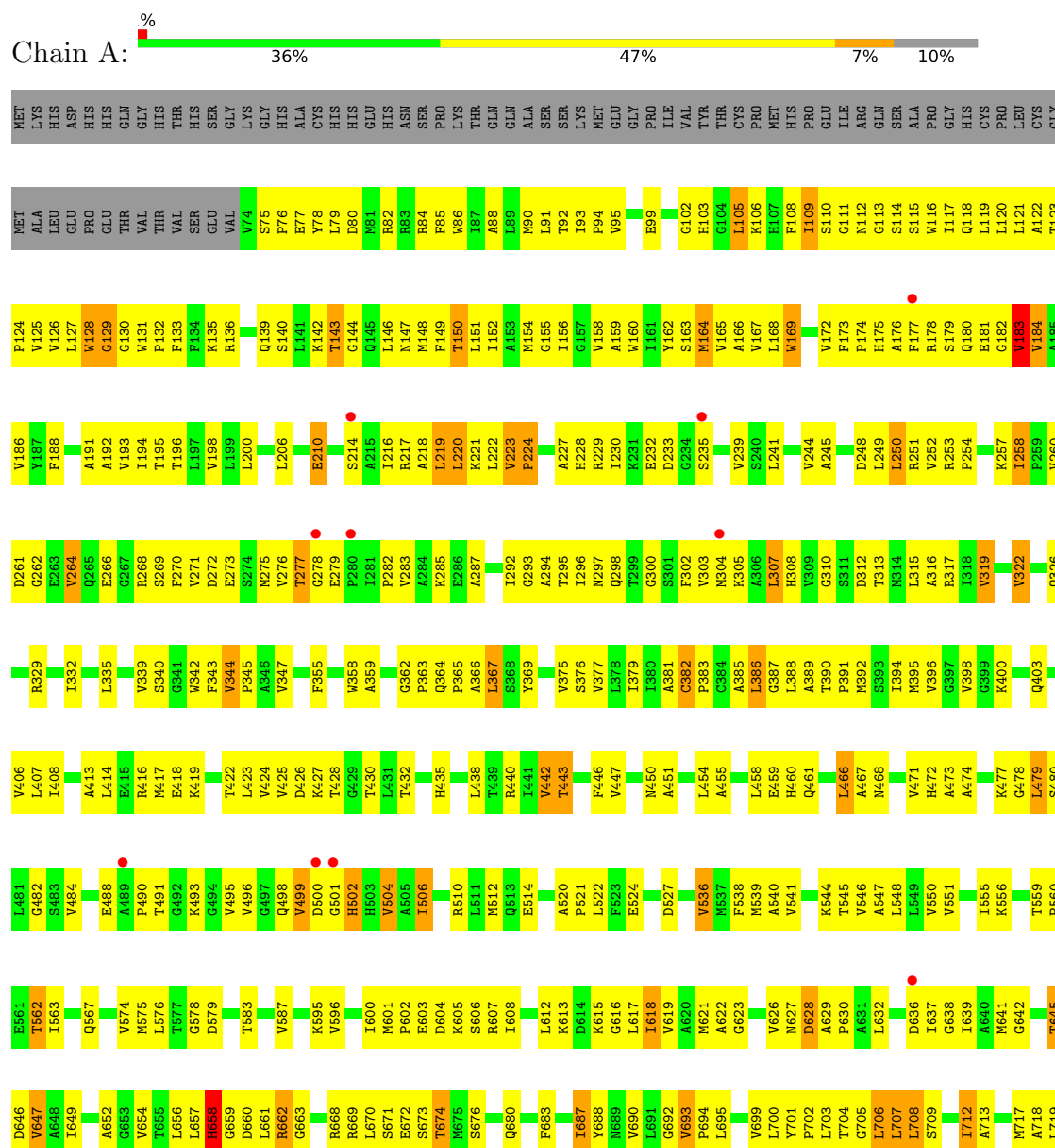
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

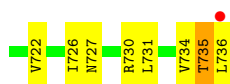
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		

3 Residue-property plots

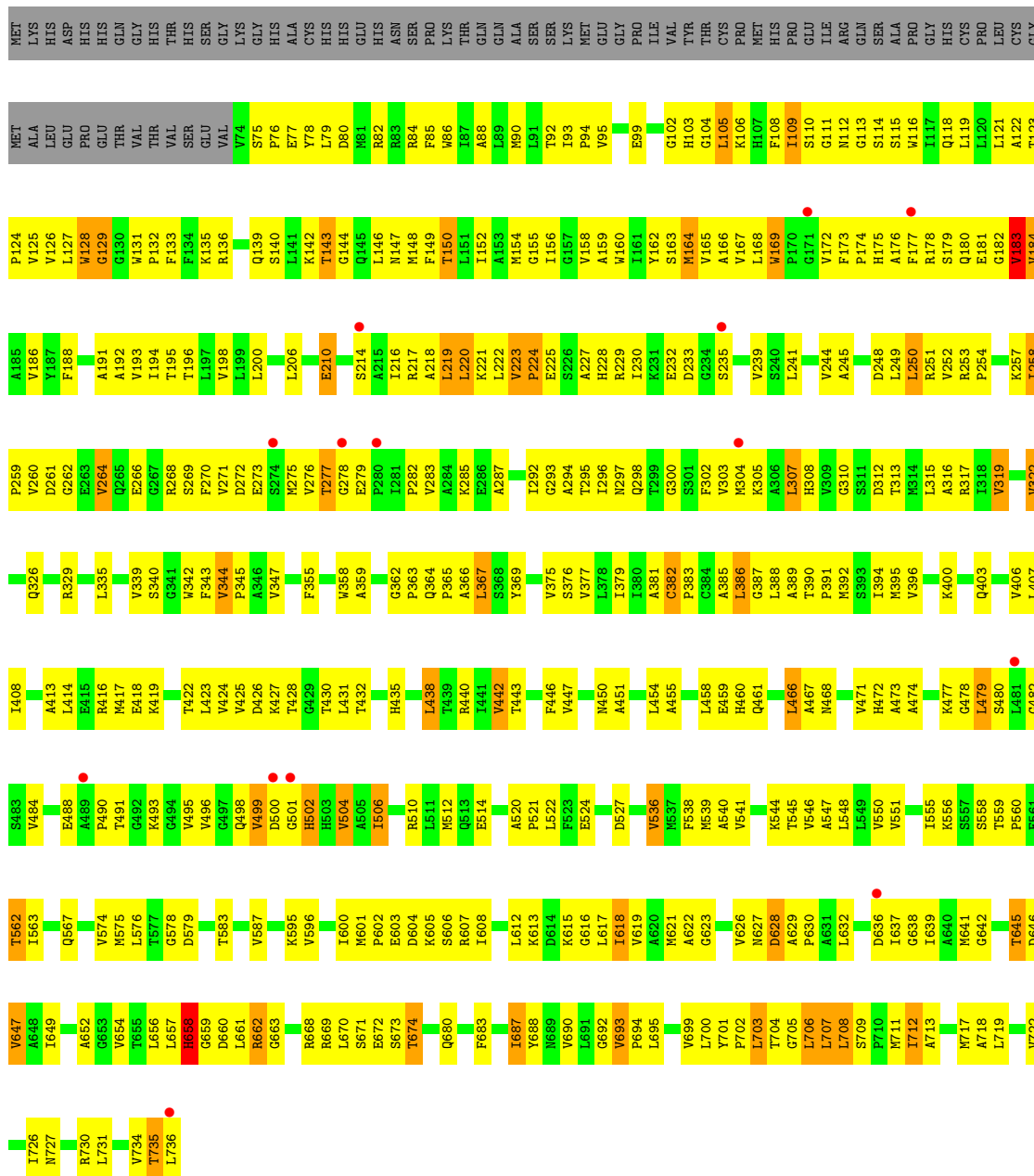
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

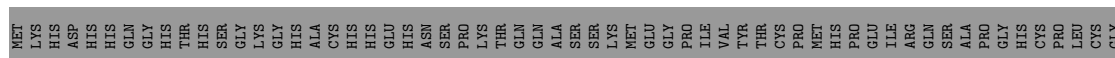


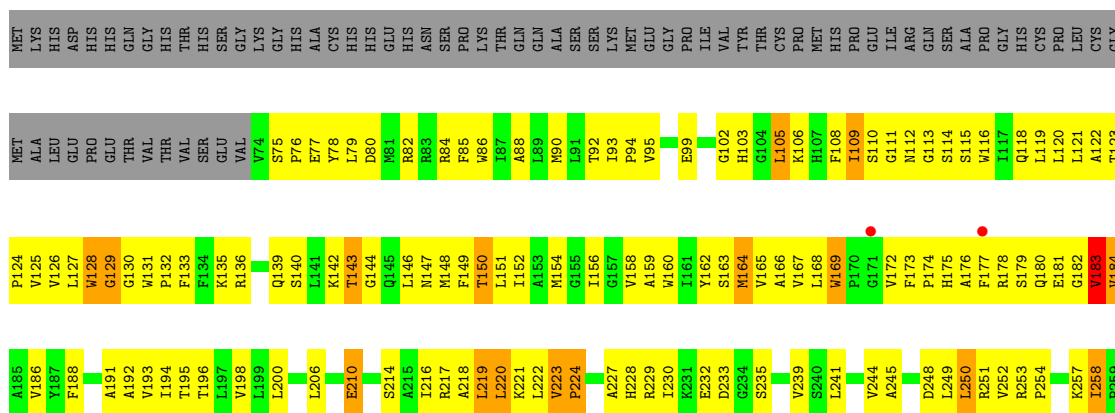


● Molecule 1: Copper efflux ATPase



● Molecule 1: Copper efflux ATPase







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.15Å 72.98Å 329.95Å 89.96° 90.04° 90.22°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-3.20) 96.5 (20.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.235 , 0.261 (Not available) , 0.252	Depositor DCC
R_{free} test set	1945 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	89.5	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 121.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l 0.428 for -h,k,-l 0.438 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19764	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: K, MG, ALF

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	0.35	0/5017	0.90	19/6812 (0.3%)
1	B	0.35	0/5017	0.90	19/6812 (0.3%)
1	C	0.35	0/5017	0.90	19/6812 (0.3%)
1	D	0.35	0/5017	0.90	19/6812 (0.3%)
All	All	0.35	0/20068	0.90	76/27248 (0.3%)

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	706	LEU	N-CA-C	8.80	118.61	108.49
1	D	706	LEU	N-CA-C	8.74	118.54	108.49
1	C	706	LEU	N-CA-C	8.73	118.53	108.49
1	A	706	LEU	N-CA-C	8.63	118.41	108.49
1	B	735	THR	N-CA-C	-7.54	103.15	111.36
1	A	735	THR	N-CA-C	-7.50	103.19	111.36
1	C	735	THR	N-CA-C	-7.50	103.19	111.36
1	D	735	THR	N-CA-C	-7.49	103.20	111.36
1	C	128	TRP	N-CA-C	-6.72	103.15	111.75
1	D	128	TRP	N-CA-C	-6.71	103.16	111.75
1	B	128	TRP	N-CA-C	-6.68	103.20	111.75
1	A	128	TRP	N-CA-C	-6.65	103.23	111.75
1	A	687	ILE	N-CA-C	6.40	117.08	110.36
1	C	687	ILE	N-CA-C	6.37	117.05	110.36
1	B	687	ILE	N-CA-C	6.31	116.98	110.36
1	D	687	ILE	N-CA-C	6.28	116.95	110.36
1	D	701	TYR	N-CA-C	-6.26	101.69	109.64
1	B	210	GLU	N-CA-C	6.23	117.76	110.97
1	B	701	TYR	N-CA-C	-6.22	101.75	109.64
1	C	701	TYR	N-CA-C	-6.21	101.75	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	TYR	N-CA-C	-6.19	101.78	109.64
1	D	210	GLU	N-CA-C	6.14	117.67	110.97
1	A	210	GLU	N-CA-C	6.07	117.59	110.97
1	C	210	GLU	N-CA-C	5.98	117.49	110.97
1	B	169	TRP	CA-C-N	5.92	126.69	120.12
1	B	169	TRP	C-N-CA	5.92	126.69	120.12
1	B	435	HIS	CA-C-N	5.92	125.83	119.85
1	B	435	HIS	C-N-CA	5.92	125.83	119.85
1	B	477	LYS	N-CA-C	-5.89	107.08	114.56
1	A	477	LYS	N-CA-C	-5.88	107.09	114.56
1	D	477	LYS	N-CA-C	-5.88	107.10	114.56
1	C	477	LYS	N-CA-C	-5.86	107.12	114.56
1	C	169	TRP	CA-C-N	5.84	126.60	120.12
1	C	169	TRP	C-N-CA	5.84	126.60	120.12
1	A	169	TRP	CA-C-N	5.74	126.50	120.12
1	A	169	TRP	C-N-CA	5.74	126.50	120.12
1	B	385	ALA	N-CA-C	5.72	117.51	111.28
1	D	169	TRP	CA-C-N	5.70	126.45	120.12
1	D	169	TRP	C-N-CA	5.70	126.45	120.12
1	B	223	VAL	CB-CA-C	-5.61	108.40	114.35
1	C	223	VAL	CB-CA-C	-5.58	108.43	114.35
1	D	223	VAL	CB-CA-C	-5.58	108.44	114.35
1	A	223	VAL	CB-CA-C	-5.55	108.47	114.35
1	D	258	ILE	CA-C-N	5.51	124.70	118.97
1	D	258	ILE	C-N-CA	5.51	124.70	118.97
1	C	435	HIS	CA-C-N	5.51	125.98	120.14
1	C	435	HIS	C-N-CA	5.51	125.98	120.14
1	A	258	ILE	CA-C-N	5.50	124.69	118.97
1	A	258	ILE	C-N-CA	5.50	124.69	118.97
1	D	435	HIS	CA-C-N	5.46	125.93	120.14
1	D	435	HIS	C-N-CA	5.46	125.93	120.14
1	A	435	HIS	CA-C-N	5.46	125.93	120.14
1	A	435	HIS	C-N-CA	5.46	125.93	120.14
1	B	258	ILE	CA-C-N	5.46	124.64	118.97
1	B	258	ILE	C-N-CA	5.46	124.64	118.97
1	C	258	ILE	CA-C-N	5.43	124.62	118.97
1	C	258	ILE	C-N-CA	5.43	124.62	118.97
1	B	502	HIS	N-CA-C	5.35	122.20	110.80
1	D	502	HIS	N-CA-C	5.32	122.13	110.80
1	C	502	HIS	N-CA-C	5.31	122.12	110.80
1	A	502	HIS	N-CA-C	5.30	122.09	110.80
1	B	706	LEU	CB-CA-C	-5.15	107.09	114.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	706	LEU	CB-CA-C	-5.15	107.09	114.87
1	A	385	ALA	N-CA-C	5.14	117.63	111.71
1	D	706	LEU	CB-CA-C	-5.14	107.11	114.87
1	C	706	LEU	CB-CA-C	-5.13	107.12	114.87
1	C	385	ALA	N-CA-C	5.10	117.57	111.71
1	D	385	ALA	N-CA-C	5.09	117.57	111.71
1	A	658	HIS	N-CA-C	5.08	121.61	110.80
1	B	658	HIS	N-CA-C	5.07	121.61	110.80
1	C	658	HIS	N-CA-C	5.07	121.60	110.80
1	D	658	HIS	N-CA-C	5.05	121.56	110.80
1	D	501	GLY	N-CA-C	-5.03	101.94	115.86
1	A	501	GLY	N-CA-C	-5.02	101.95	115.86
1	B	501	GLY	N-CA-C	-5.02	101.96	115.86
1	C	501	GLY	N-CA-C	-5.00	102.00	115.86

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	4934	0	5125	408	0
1	B	4934	0	5125	416	0
1	C	4934	0	5125	416	0
1	D	4934	0	5125	406	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
All	All	19764	0	20500	1634	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 (1634) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:THR:HG23	1:B:124:PRO:HD3	1.31	1.12
1:C:123:THR:HG23	1:C:124:PRO:HD3	1.31	1.12
1:A:123:THR:HG23	1:A:124:PRO:HD3	1.31	1.12
1:D:123:THR:HG23	1:D:124:PRO:HD3	1.31	1.12
1:A:662:ARG:HB2	1:A:663:GLY:HA3	1.34	1.09
1:D:662:ARG:HB2	1:D:663:GLY:HA3	1.34	1.09
1:B:662:ARG:HB2	1:B:663:GLY:HA3	1.34	1.09
1:C:662:ARG:HB2	1:C:663:GLY:HA3	1.35	1.08
1:D:112:ASN:O	1:D:116:TRP:HB2	1.55	1.06
1:A:112:ASN:O	1:A:116:TRP:HB2	1.55	1.06
1:B:112:ASN:O	1:B:116:TRP:HB2	1.54	1.05
1:C:112:ASN:O	1:C:116:TRP:HB2	1.54	1.05
1:C:264:VAL:HA	1:C:303:VAL:O	1.57	1.04
1:B:264:VAL:HA	1:B:303:VAL:O	1.57	1.04
1:A:264:VAL:HA	1:A:303:VAL:O	1.57	1.02
1:D:264:VAL:HA	1:D:303:VAL:O	1.57	1.02
1:C:109:ILE:HG23	1:C:110:SER:HB3	1.41	1.00
1:B:109:ILE:HG23	1:B:110:SER:HB3	1.42	0.99
1:D:109:ILE:HG23	1:D:110:SER:HB3	1.43	0.96
1:A:109:ILE:HG23	1:A:110:SER:HB3	1.43	0.96
1:D:178:ARG:HB3	1:D:179:SER:HA	1.47	0.94
1:A:178:ARG:HB3	1:A:179:SER:HA	1.46	0.94
1:C:178:ARG:HB3	1:C:179:SER:HA	1.47	0.94
1:A:102:GLY:HA3	1:A:103:HIS:C	1.92	0.94
1:B:178:ARG:HB3	1:B:179:SER:HA	1.47	0.94
1:D:102:GLY:HA3	1:D:103:HIS:C	1.92	0.93
1:B:102:GLY:HA3	1:B:103:HIS:C	1.93	0.92
1:C:102:GLY:HA3	1:C:103:HIS:C	1.92	0.92
1:A:123:THR:CG2	1:A:124:PRO:HD3	2.04	0.88
1:D:123:THR:CG2	1:D:124:PRO:HD3	2.04	0.88
1:C:123:THR:CG2	1:C:124:PRO:HD3	2.03	0.87
1:B:123:THR:CG2	1:B:124:PRO:HD3	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:C	1:B:224:PRO:HD2	2.01	0.85
1:C:222:LEU:C	1:C:224:PRO:HD2	2.02	0.85
1:B:482:GLY:HA3	1:B:499:VAL:HG23	1.58	0.85
1:C:482:GLY:HA3	1:C:499:VAL:HG23	1.59	0.85
1:A:222:LEU:C	1:A:224:PRO:HD2	2.02	0.85
1:D:222:LEU:C	1:D:224:PRO:HD2	2.02	0.85
1:A:482:GLY:HA3	1:A:499:VAL:HG23	1.59	0.84
1:D:482:GLY:HA3	1:D:499:VAL:HG23	1.59	0.84
1:D:229:ARG:HG2	1:D:250:LEU:HD21	1.60	0.83
1:A:229:ARG:HG2	1:A:250:LEU:HD21	1.60	0.83
1:A:416:ARG:HB2	1:A:637:ILE:HD11	1.60	0.83
1:D:416:ARG:HB2	1:D:637:ILE:HD11	1.59	0.83
1:C:229:ARG:HG2	1:C:250:LEU:HD21	1.60	0.82
1:B:229:ARG:HG2	1:B:250:LEU:HD21	1.60	0.82
1:D:451:ALA:HB1	1:D:539:MET:HE1	1.62	0.82
1:C:416:ARG:HB2	1:C:637:ILE:HD11	1.59	0.82
1:B:416:ARG:HB2	1:B:637:ILE:HD11	1.59	0.82
1:B:232:GLU:HG3	1:B:233:ASP:H	1.43	0.81
1:C:232:GLU:HG3	1:C:233:ASP:H	1.43	0.81
1:A:451:ALA:HB1	1:A:539:MET:HE1	1.63	0.81
1:A:563:ILE:O	1:A:567:GLN:HG2	1.81	0.81
1:D:563:ILE:O	1:D:567:GLN:HG2	1.81	0.81
1:D:232:GLU:HG3	1:D:233:ASP:H	1.43	0.81
1:A:232:GLU:HG3	1:A:233:ASP:H	1.43	0.80
1:B:563:ILE:O	1:B:567:GLN:HG2	1.81	0.80
1:C:563:ILE:O	1:C:567:GLN:HG2	1.81	0.80
1:D:662:ARG:HB2	1:D:663:GLY:CA	2.11	0.80
1:B:451:ALA:HB1	1:B:539:MET:HE1	1.62	0.80
1:A:662:ARG:HB2	1:A:663:GLY:CA	2.12	0.80
1:D:254:PRO:HB3	1:D:300:GLY:H	1.47	0.80
1:B:662:ARG:HB2	1:B:663:GLY:CA	2.11	0.79
1:A:254:PRO:HB3	1:A:300:GLY:H	1.48	0.79
1:C:662:ARG:HB2	1:C:663:GLY:CA	2.12	0.79
1:D:708:LEU:HD21	1:D:712:ILE:HD11	1.63	0.79
1:C:254:PRO:HB3	1:C:300:GLY:H	1.47	0.79
1:A:708:LEU:HD21	1:A:712:ILE:HD11	1.64	0.78
1:B:254:PRO:HB3	1:B:300:GLY:H	1.48	0.78
1:C:451:ALA:HB1	1:C:539:MET:HE1	1.63	0.78
1:C:708:LEU:HD21	1:C:712:ILE:HD11	1.63	0.78
1:B:119:LEU:O	1:B:123:THR:HG22	1.84	0.78
1:B:708:LEU:HD21	1:B:712:ILE:HD11	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:THR:HG21	1:B:623:GLY:HA2	1.66	0.77
1:B:604:ASP:O	1:B:608:ILE:HG12	1.84	0.77
1:C:604:ASP:O	1:C:608:ILE:HG12	1.85	0.77
1:C:119:LEU:O	1:C:123:THR:HG22	1.85	0.77
1:C:430:THR:HG21	1:C:623:GLY:HA2	1.67	0.77
1:A:119:LEU:O	1:A:123:THR:HG22	1.84	0.77
1:D:119:LEU:O	1:D:123:THR:HG22	1.84	0.77
1:D:499:VAL:HG22	1:D:500:ASP:H	1.49	0.77
1:B:499:VAL:HG22	1:B:500:ASP:H	1.49	0.77
1:B:430:THR:HA	1:B:641:MET:HE2	1.67	0.76
1:D:430:THR:HG21	1:D:623:GLY:HA2	1.66	0.76
1:A:499:VAL:HG22	1:A:500:ASP:H	1.49	0.76
1:C:430:THR:HA	1:C:641:MET:HE2	1.67	0.76
1:C:499:VAL:HG22	1:C:500:ASP:H	1.49	0.76
1:A:430:THR:HG21	1:A:623:GLY:HA2	1.66	0.76
1:D:604:ASP:O	1:D:608:ILE:HG12	1.84	0.76
1:A:124:PRO:O	1:A:128:TRP:HB3	1.85	0.76
1:A:604:ASP:O	1:A:608:ILE:HG12	1.84	0.76
1:B:662:ARG:CB	1:B:663:GLY:HA3	2.14	0.76
1:C:662:ARG:CB	1:C:663:GLY:HA3	2.14	0.76
1:D:124:PRO:O	1:D:128:TRP:HB3	1.86	0.75
1:A:430:THR:HA	1:A:641:MET:HE2	1.66	0.75
1:A:335:LEU:O	1:A:339:VAL:HG12	1.87	0.75
1:D:335:LEU:O	1:D:339:VAL:HG12	1.87	0.75
1:B:124:PRO:O	1:B:128:TRP:HB3	1.86	0.74
1:C:124:PRO:O	1:C:128:TRP:HB3	1.86	0.74
1:C:232:GLU:CG	1:C:233:ASP:H	2.00	0.74
1:D:430:THR:HA	1:D:641:MET:HE2	1.66	0.74
1:B:232:GLU:CG	1:B:233:ASP:H	2.00	0.74
1:B:159:ALA:HB2	1:B:379:ILE:HD13	1.68	0.74
1:D:232:GLU:CG	1:D:233:ASP:H	2.00	0.74
1:A:232:GLU:CG	1:A:233:ASP:H	2.00	0.74
1:B:78:TYR:HD2	1:B:79:LEU:HD12	1.53	0.74
1:D:662:ARG:CB	1:D:663:GLY:HA3	2.14	0.74
1:B:335:LEU:O	1:B:339:VAL:HG12	1.87	0.74
1:C:78:TYR:HD2	1:C:79:LEU:HD12	1.53	0.74
1:A:662:ARG:CB	1:A:663:GLY:HA3	2.14	0.73
1:C:159:ALA:HB2	1:C:379:ILE:HD13	1.68	0.73
1:C:147:ASN:H	1:C:150:THR:HG23	1.53	0.73
1:D:110:SER:HB2	1:D:114:SER:HB3	1.69	0.73
1:D:159:ALA:HB2	1:D:379:ILE:HD13	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:SER:HB2	1:A:114:SER:HB3	1.69	0.73
1:C:335:LEU:O	1:C:339:VAL:HG12	1.87	0.73
1:B:147:ASN:H	1:B:150:THR:HG23	1.53	0.73
1:C:88:ALA:HB1	1:C:196:THR:HG22	1.70	0.73
1:C:110:SER:HB2	1:C:114:SER:HB3	1.69	0.73
1:B:110:SER:HB2	1:B:114:SER:HB3	1.70	0.72
1:C:152:ILE:HA	1:C:382:CYS:SG	2.29	0.72
1:B:88:ALA:HB1	1:B:196:THR:HG22	1.71	0.72
1:D:615:LYS:HG3	1:D:616:GLY:H	1.54	0.72
1:A:159:ALA:HB2	1:A:379:ILE:HD13	1.69	0.72
1:B:152:ILE:HA	1:B:382:CYS:SG	2.29	0.72
1:A:152:ILE:HA	1:A:382:CYS:SG	2.29	0.72
1:A:615:LYS:HG3	1:A:616:GLY:H	1.55	0.72
1:A:78:TYR:HD2	1:A:79:LEU:HD12	1.53	0.72
1:A:147:ASN:H	1:A:150:THR:HG23	1.53	0.72
1:D:147:ASN:H	1:D:150:THR:HG23	1.53	0.72
1:D:700:LEU:HB3	1:D:704:THR:OG1	1.88	0.72
1:C:700:LEU:HB3	1:C:704:THR:OG1	1.88	0.72
1:D:78:TYR:HD2	1:D:79:LEU:HD12	1.53	0.72
1:C:418:GLU:HG3	1:C:672:GLU:HG2	1.70	0.71
1:D:418:GLU:HG3	1:D:672:GLU:HG2	1.70	0.71
1:A:418:GLU:HG3	1:A:672:GLU:HG2	1.70	0.71
1:B:418:GLU:HG3	1:B:672:GLU:HG2	1.70	0.71
1:C:615:LYS:HG3	1:C:616:GLY:H	1.54	0.71
1:B:608:ILE:O	1:B:612:LEU:HD23	1.90	0.71
1:B:700:LEU:HB3	1:B:704:THR:OG1	1.88	0.71
1:A:413:ALA:HA	1:A:637:ILE:HD12	1.72	0.71
1:B:140:SER:OG	1:B:150:THR:HG22	1.89	0.71
1:B:175:HIS:HB2	1:B:176:ALA:HA	1.71	0.71
1:C:175:HIS:HB2	1:C:176:ALA:HA	1.71	0.71
1:D:152:ILE:HA	1:D:382:CYS:SG	2.30	0.71
1:A:140:SER:OG	1:A:150:THR:HG22	1.90	0.71
1:B:615:LYS:HG3	1:B:616:GLY:H	1.55	0.71
1:C:608:ILE:O	1:C:612:LEU:HD23	1.90	0.71
1:A:88:ALA:HB1	1:A:196:THR:HG22	1.71	0.71
1:A:700:LEU:HB3	1:A:704:THR:OG1	1.89	0.71
1:C:140:SER:OG	1:C:150:THR:HG22	1.90	0.71
1:A:175:HIS:HB2	1:A:176:ALA:HA	1.72	0.71
1:C:160:TRP:O	1:C:164:MET:HB2	1.91	0.71
1:D:140:SER:OG	1:D:150:THR:HG22	1.90	0.71
1:D:175:HIS:HB2	1:D:176:ALA:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:ALA:HA	1:D:637:ILE:HD12	1.72	0.71
1:B:160:TRP:O	1:B:164:MET:HB2	1.91	0.71
1:D:687:ILE:HA	1:D:690:VAL:HG12	1.73	0.71
1:A:688:TYR:CD1	1:A:719:LEU:HD23	2.26	0.71
1:A:249:LEU:O	1:A:250:LEU:HD23	1.91	0.70
1:D:249:LEU:O	1:D:250:LEU:HD23	1.92	0.70
1:C:688:TYR:CD1	1:C:719:LEU:HD23	2.26	0.70
1:C:413:ALA:HA	1:C:637:ILE:HD12	1.72	0.70
1:D:608:ILE:O	1:D:612:LEU:HD23	1.90	0.70
1:A:687:ILE:HA	1:A:690:VAL:HG12	1.74	0.70
1:C:556:LYS:HB2	1:C:559:THR:OG1	1.92	0.70
1:D:254:PRO:HB3	1:D:300:GLY:N	2.07	0.70
1:A:254:PRO:HB3	1:A:300:GLY:N	2.07	0.70
1:B:413:ALA:HA	1:B:637:ILE:HD12	1.72	0.70
1:C:687:ILE:HA	1:C:690:VAL:HG12	1.74	0.70
1:D:121:LEU:O	1:D:124:PRO:HD2	1.92	0.70
1:B:283:VAL:HG23	1:B:285:LYS:HE2	1.74	0.70
1:B:556:LYS:HB2	1:B:559:THR:OG1	1.92	0.70
1:B:687:ILE:HA	1:B:690:VAL:HG12	1.74	0.70
1:C:432:THR:HG22	1:C:555:ILE:HA	1.74	0.70
1:A:432:THR:HG22	1:A:555:ILE:HA	1.74	0.70
1:B:194:ILE:O	1:B:198:VAL:HG12	1.92	0.70
1:B:432:THR:HG22	1:B:555:ILE:HA	1.74	0.70
1:C:283:VAL:HG23	1:C:285:LYS:HE2	1.74	0.70
1:A:608:ILE:O	1:A:612:LEU:HD23	1.91	0.69
1:C:254:PRO:HB3	1:C:300:GLY:N	2.07	0.69
1:D:160:TRP:O	1:D:164:MET:HB2	1.91	0.69
1:D:432:THR:HG22	1:D:555:ILE:HA	1.74	0.69
1:A:160:TRP:O	1:A:164:MET:HB2	1.91	0.69
1:B:254:PRO:HB3	1:B:300:GLY:N	2.07	0.69
1:C:661:LEU:O	1:C:661:LEU:HD23	1.92	0.69
1:D:93:ILE:HG23	1:D:94:PRO:HD3	1.75	0.69
1:C:121:LEU:O	1:C:124:PRO:HD2	1.92	0.69
1:C:249:LEU:O	1:C:250:LEU:HD23	1.91	0.69
1:D:688:TYR:CD1	1:D:719:LEU:HD23	2.28	0.69
1:A:93:ILE:HG23	1:A:94:PRO:HD3	1.75	0.69
1:D:661:LEU:HD23	1:D:661:LEU:O	1.92	0.69
1:B:249:LEU:O	1:B:250:LEU:HD23	1.91	0.69
1:B:688:TYR:CD1	1:B:719:LEU:HD23	2.27	0.69
1:D:88:ALA:HB1	1:D:196:THR:HG22	1.72	0.69
1:D:122:ALA:HA	1:D:125:VAL:HG12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ILE:O	1:C:198:VAL:HG12	1.92	0.69
1:D:194:ILE:O	1:D:198:VAL:HG12	1.92	0.69
1:A:122:ALA:HA	1:A:125:VAL:HG12	1.74	0.69
1:A:556:LYS:HB2	1:A:559:THR:OG1	1.91	0.69
1:A:661:LEU:O	1:A:661:LEU:HD23	1.92	0.69
1:B:121:LEU:O	1:B:124:PRO:HD2	1.93	0.69
1:C:122:ALA:HA	1:C:125:VAL:HG12	1.74	0.69
1:A:194:ILE:O	1:A:198:VAL:HG12	1.93	0.69
1:B:122:ALA:HA	1:B:125:VAL:HG12	1.75	0.69
1:B:661:LEU:HD23	1:B:661:LEU:O	1.93	0.69
1:A:121:LEU:O	1:A:124:PRO:HD2	1.93	0.68
1:B:93:ILE:HG23	1:B:94:PRO:HD3	1.75	0.68
1:B:223:VAL:O	1:B:224:PRO:C	2.37	0.68
1:C:223:VAL:O	1:C:224:PRO:C	2.37	0.68
1:A:283:VAL:HG23	1:A:285:LYS:HE2	1.74	0.68
1:D:283:VAL:HG23	1:D:285:LYS:HE2	1.74	0.68
1:B:273:GLU:O	1:B:273:GLU:HG2	1.93	0.68
1:C:93:ILE:HG23	1:C:94:PRO:HD3	1.76	0.68
1:C:273:GLU:O	1:C:273:GLU:HG2	1.94	0.68
1:C:377:VAL:HG23	1:C:693:VAL:HB	1.75	0.68
1:B:520:ALA:HB3	1:B:521:PRO:HD3	1.76	0.68
1:D:556:LYS:HB2	1:D:559:THR:OG1	1.92	0.68
1:D:273:GLU:O	1:D:273:GLU:HG2	1.93	0.68
1:A:273:GLU:O	1:A:273:GLU:HG2	1.93	0.67
1:D:223:VAL:O	1:D:224:PRO:C	2.37	0.67
1:A:223:VAL:O	1:A:224:PRO:C	2.37	0.67
1:B:541:VAL:HG22	1:B:546:VAL:HG11	1.77	0.67
1:C:520:ALA:HB3	1:C:521:PRO:HD3	1.76	0.67
1:A:108:PHE:O	1:A:109:ILE:HD12	1.95	0.67
1:B:377:VAL:HG23	1:B:693:VAL:HB	1.76	0.67
1:A:377:VAL:HG23	1:A:693:VAL:HB	1.75	0.67
1:A:520:ALA:HB3	1:A:521:PRO:HD3	1.76	0.67
1:C:541:VAL:HG22	1:C:546:VAL:HG11	1.77	0.67
1:D:108:PHE:O	1:D:109:ILE:HD12	1.95	0.67
1:C:110:SER:HA	1:C:114:SER:H	1.60	0.67
1:A:110:SER:HA	1:A:114:SER:H	1.60	0.67
1:D:377:VAL:HG23	1:D:693:VAL:HB	1.76	0.67
1:D:520:ALA:HB3	1:D:521:PRO:HD3	1.77	0.66
1:B:307:LEU:HD13	1:B:308:HIS:HD2	1.61	0.66
1:B:687:ILE:HD13	1:D:120:LEU:HD12	1.76	0.66
1:D:541:VAL:HG22	1:D:546:VAL:HG11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LEU:HD13	1:A:308:HIS:HD2	1.60	0.66
1:C:307:LEU:HD13	1:C:308:HIS:HD2	1.61	0.66
1:A:541:VAL:HG22	1:A:546:VAL:HG11	1.77	0.66
1:B:108:PHE:O	1:B:109:ILE:HD12	1.95	0.66
1:D:110:SER:HA	1:D:114:SER:H	1.61	0.66
1:B:110:SER:HA	1:B:114:SER:H	1.61	0.66
1:C:108:PHE:O	1:C:109:ILE:HD12	1.96	0.66
1:A:179:SER:HB2	1:A:183:VAL:N	2.11	0.66
1:D:307:LEU:HD13	1:D:308:HIS:HD2	1.61	0.66
1:D:179:SER:HB2	1:D:183:VAL:N	2.11	0.65
1:C:179:SER:HB2	1:C:183:VAL:N	2.11	0.65
1:A:605:LYS:HE2	1:A:628:ASP:HB3	1.79	0.65
1:D:605:LYS:HE2	1:D:628:ASP:HB3	1.79	0.65
1:A:490:PRO:HB2	1:A:493:LYS:HD3	1.79	0.65
1:B:179:SER:HB2	1:B:183:VAL:N	2.11	0.65
1:B:605:LYS:HE2	1:B:628:ASP:HB3	1.78	0.65
1:D:192:ALA:O	1:D:196:THR:HG23	1.96	0.65
1:D:490:PRO:HB2	1:D:493:LYS:HD3	1.79	0.64
1:A:192:ALA:O	1:A:196:THR:HG23	1.96	0.64
1:B:192:ALA:O	1:B:196:THR:HG23	1.98	0.64
1:C:192:ALA:O	1:C:196:THR:HG23	1.98	0.64
1:C:490:PRO:HB2	1:C:493:LYS:HD3	1.79	0.64
1:C:605:LYS:HE2	1:C:628:ASP:HB3	1.78	0.64
1:C:670:LEU:HD23	1:C:736:LEU:HD11	1.79	0.64
1:A:93:ILE:CG2	1:A:94:PRO:HD3	2.27	0.64
1:A:417:MET:HE2	1:A:637:ILE:HG21	1.78	0.64
1:B:112:ASN:O	1:B:116:TRP:CB	2.40	0.64
1:B:490:PRO:HB2	1:B:493:LYS:HD3	1.79	0.64
1:D:93:ILE:CG2	1:D:94:PRO:HD3	2.27	0.64
1:C:417:MET:HE2	1:C:637:ILE:HG21	1.78	0.64
1:A:670:LEU:O	1:A:674:THR:HG23	1.98	0.64
1:C:112:ASN:O	1:C:116:TRP:CB	2.40	0.64
1:B:417:MET:HE2	1:B:637:ILE:HG21	1.79	0.64
1:D:670:LEU:O	1:D:674:THR:HG23	1.98	0.64
1:B:506:ILE:HD12	1:B:538:PHE:O	1.98	0.64
1:A:111:GLY:O	1:A:115:SER:HB2	1.98	0.63
1:D:417:MET:HE2	1:D:637:ILE:HG21	1.79	0.63
1:B:111:GLY:O	1:B:115:SER:HB2	1.98	0.63
1:B:670:LEU:HD23	1:B:736:LEU:HD11	1.80	0.63
1:B:93:ILE:CG2	1:B:94:PRO:HD3	2.28	0.63
1:C:93:ILE:CG2	1:C:94:PRO:HD3	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:GLY:O	1:D:115:SER:HB2	1.98	0.63
1:C:109:ILE:CG2	1:C:110:SER:HB3	2.22	0.63
1:C:506:ILE:HD12	1:C:538:PHE:O	1.99	0.63
1:A:670:LEU:HD23	1:A:736:LEU:HD11	1.79	0.63
1:C:111:GLY:O	1:C:115:SER:HB2	1.98	0.63
1:A:506:ILE:HD12	1:A:538:PHE:O	1.98	0.63
1:D:506:ILE:HD12	1:D:538:PHE:O	1.98	0.63
1:B:109:ILE:CG2	1:B:110:SER:HB3	2.23	0.63
1:C:670:LEU:O	1:C:674:THR:HG23	1.98	0.63
1:D:670:LEU:HD23	1:D:736:LEU:HD11	1.79	0.63
1:B:670:LEU:O	1:B:674:THR:HG23	1.98	0.62
1:A:105:LEU:HD12	1:A:106:LYS:N	2.14	0.62
1:C:454:LEU:HD21	1:C:500:ASP:OD1	1.99	0.62
1:D:105:LEU:HD12	1:D:106:LYS:N	2.15	0.62
1:C:223:VAL:N	1:C:224:PRO:HD2	2.14	0.62
1:C:342:TRP:O	1:C:345:PRO:HD2	2.00	0.62
1:B:216:ILE:O	1:B:219:LEU:HD13	2.00	0.62
1:B:223:VAL:N	1:B:224:PRO:HD2	2.14	0.62
1:A:315:LEU:O	1:A:319:VAL:HG12	2.00	0.62
1:B:454:LEU:HD21	1:B:500:ASP:OD1	2.00	0.62
1:C:216:ILE:O	1:C:219:LEU:HD13	2.00	0.62
1:C:423:LEU:HG	1:C:425:VAL:HG13	1.81	0.62
1:C:105:LEU:HD12	1:C:106:LYS:N	2.14	0.62
1:C:315:LEU:O	1:C:319:VAL:HG12	1.99	0.62
1:D:109:ILE:CG2	1:D:110:SER:HB3	2.23	0.62
1:D:315:LEU:O	1:D:319:VAL:HG12	2.00	0.62
1:A:109:ILE:CG2	1:A:110:SER:HB3	2.23	0.61
1:A:454:LEU:HD21	1:A:500:ASP:OD1	2.00	0.61
1:B:105:LEU:HD12	1:B:106:LYS:N	2.14	0.61
1:D:216:ILE:O	1:D:219:LEU:HD13	2.00	0.61
1:D:342:TRP:O	1:D:345:PRO:HD2	2.00	0.61
1:A:178:ARG:CB	1:A:179:SER:HA	2.24	0.61
1:A:216:ILE:HG23	1:A:217:ARG:H	1.66	0.61
1:A:216:ILE:O	1:A:219:LEU:HD13	2.00	0.61
1:D:216:ILE:HG23	1:D:217:ARG:H	1.66	0.61
1:D:454:LEU:HD21	1:D:500:ASP:OD1	2.00	0.61
1:B:342:TRP:O	1:B:345:PRO:HD2	2.00	0.61
1:B:418:GLU:HB2	1:B:671:SER:OG	2.00	0.61
1:B:315:LEU:O	1:B:319:VAL:HG12	2.00	0.61
1:B:423:LEU:HG	1:B:425:VAL:HG13	1.81	0.61
1:C:629:ALA:N	1:C:630:PRO:HD2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:VAL:N	1:D:224:PRO:HD2	2.15	0.61
1:A:142:LYS:HG2	1:A:143:THR:HG23	1.82	0.61
1:A:223:VAL:N	1:A:224:PRO:HD2	2.14	0.61
1:B:629:ALA:N	1:B:630:PRO:HD2	2.16	0.61
1:D:142:LYS:HG2	1:D:143:THR:HG23	1.82	0.61
1:A:342:TRP:O	1:A:345:PRO:HD2	2.01	0.61
1:D:178:ARG:CB	1:D:179:SER:HA	2.24	0.61
1:A:423:LEU:HG	1:A:425:VAL:HG13	1.81	0.61
1:C:142:LYS:HG2	1:C:143:THR:HG23	1.82	0.61
1:D:418:GLU:HB2	1:D:671:SER:OG	2.00	0.61
1:D:629:ALA:N	1:D:630:PRO:HD2	2.15	0.61
1:A:120:LEU:HD12	1:C:687:ILE:HD13	1.82	0.61
1:A:629:ALA:N	1:A:630:PRO:HD2	2.16	0.61
1:B:142:LYS:HG2	1:B:143:THR:HG23	1.82	0.61
1:B:179:SER:HB3	1:B:181:GLU:N	2.16	0.60
1:C:344:VAL:HG22	1:C:345:PRO:HD3	1.82	0.60
1:C:418:GLU:HB2	1:C:671:SER:OG	2.01	0.60
1:B:262:GLY:HA2	1:B:307:LEU:HB2	1.83	0.60
1:B:662:ARG:CB	1:B:663:GLY:CA	2.77	0.60
1:C:179:SER:HB3	1:C:181:GLU:N	2.16	0.60
1:D:166:ALA:HA	1:D:173:PHE:HE2	1.66	0.60
1:D:423:LEU:HG	1:D:425:VAL:HG13	1.82	0.60
1:A:166:ALA:HA	1:A:173:PHE:HE2	1.65	0.60
1:C:166:ALA:HA	1:C:173:PHE:HE2	1.65	0.60
1:C:262:GLY:HA2	1:C:307:LEU:HB2	1.83	0.60
1:C:662:ARG:CB	1:C:663:GLY:CA	2.78	0.60
1:C:709:SER:O	1:C:712:ILE:HG13	2.01	0.60
1:B:216:ILE:HG23	1:B:217:ARG:H	1.66	0.60
1:C:216:ILE:HG23	1:C:217:ARG:H	1.66	0.60
1:D:709:SER:O	1:D:712:ILE:HG13	2.02	0.60
1:B:191:ALA:O	1:B:195:THR:HG23	2.02	0.60
1:B:344:VAL:HG22	1:B:345:PRO:HD3	1.83	0.60
1:B:709:SER:O	1:B:712:ILE:HG13	2.01	0.60
1:A:709:SER:O	1:A:712:ILE:HG13	2.02	0.60
1:B:166:ALA:HA	1:B:173:PHE:HE2	1.66	0.60
1:A:344:VAL:HG22	1:A:345:PRO:HD3	1.83	0.60
1:A:418:GLU:HB2	1:A:671:SER:OG	2.01	0.60
1:A:179:SER:HB3	1:A:181:GLU:N	2.17	0.59
1:D:262:GLY:HA2	1:D:307:LEU:HB2	1.83	0.59
1:D:179:SER:HB3	1:D:181:GLU:N	2.17	0.59
1:D:344:VAL:HG22	1:D:345:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASN:O	1:A:116:TRP:CB	2.40	0.59
1:A:262:GLY:HA2	1:A:307:LEU:HB2	1.83	0.59
1:A:275:MET:HE1	1:A:294:ALA:HB3	1.85	0.59
1:B:683:PHE:CZ	1:B:687:ILE:HD12	2.37	0.59
1:C:683:PHE:CZ	1:C:687:ILE:HD12	2.37	0.59
1:D:275:MET:HE1	1:D:294:ALA:HB3	1.85	0.59
1:A:646:ASP:O	1:A:649:ILE:HG22	2.03	0.59
1:B:499:VAL:HG22	1:B:500:ASP:N	2.18	0.59
1:B:466:LEU:HD21	1:B:551:VAL:HG21	1.85	0.59
1:C:707:LEU:HD22	1:C:707:LEU:C	2.28	0.59
1:D:112:ASN:O	1:D:116:TRP:CB	2.40	0.59
1:D:191:ALA:O	1:D:195:THR:HG23	2.03	0.59
1:B:268:ARG:HE	1:B:491:THR:HG21	1.68	0.59
1:C:268:ARG:HE	1:C:491:THR:HG21	1.68	0.59
1:A:712:ILE:C	1:A:712:ILE:HD12	2.28	0.58
1:B:707:LEU:C	1:B:707:LEU:HD22	2.28	0.58
1:C:499:VAL:HG22	1:C:500:ASP:N	2.18	0.58
1:D:646:ASP:O	1:D:649:ILE:HG22	2.03	0.58
1:A:683:PHE:CZ	1:A:687:ILE:HD12	2.37	0.58
1:C:121:LEU:C	1:C:124:PRO:HD2	2.28	0.58
1:C:646:ASP:O	1:C:649:ILE:HG22	2.03	0.58
1:D:268:ARG:HE	1:D:491:THR:HG21	1.68	0.58
1:B:121:LEU:C	1:B:124:PRO:HD2	2.29	0.58
1:D:400:LYS:O	1:D:403:GLN:HB3	2.04	0.58
1:D:662:ARG:CB	1:D:663:GLY:CA	2.77	0.58
1:C:466:LEU:HD21	1:C:551:VAL:HG21	1.86	0.58
1:D:683:PHE:CZ	1:D:687:ILE:HD12	2.38	0.58
1:A:147:ASN:H	1:A:150:THR:CG2	2.16	0.58
1:A:268:ARG:HE	1:A:491:THR:HG21	1.68	0.58
1:B:712:ILE:HD12	1:B:712:ILE:C	2.28	0.58
1:C:191:ALA:O	1:C:195:THR:HG23	2.04	0.58
1:A:191:ALA:O	1:A:195:THR:HG23	2.04	0.58
1:A:400:LYS:O	1:A:403:GLN:HB3	2.04	0.58
1:A:447:VAL:CG2	1:A:450:ASN:HB2	2.34	0.58
1:A:662:ARG:CB	1:A:663:GLY:CA	2.77	0.58
1:A:707:LEU:C	1:A:707:LEU:HD22	2.28	0.58
1:D:712:ILE:C	1:D:712:ILE:HD12	2.28	0.58
1:B:400:LYS:O	1:B:403:GLN:HB3	2.04	0.58
1:B:499:VAL:O	1:B:502:HIS:CG	2.56	0.58
1:C:275:MET:HE1	1:C:294:ALA:HB3	1.85	0.58
1:C:400:LYS:O	1:C:403:GLN:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:VAL:CG2	1:D:450:ASN:HB2	2.34	0.58
1:D:466:LEU:HD21	1:D:551:VAL:HG21	1.85	0.58
1:C:499:VAL:O	1:C:502:HIS:CG	2.56	0.58
1:D:147:ASN:H	1:D:150:THR:CG2	2.16	0.58
1:D:707:LEU:C	1:D:707:LEU:HD22	2.28	0.58
1:B:275:MET:HE1	1:B:294:ALA:HB3	1.85	0.57
1:D:119:LEU:HD12	1:D:167:VAL:HG11	1.86	0.57
1:D:499:VAL:HG22	1:D:500:ASP:N	2.18	0.57
1:D:499:VAL:O	1:D:502:HIS:CG	2.56	0.57
1:D:414:LEU:HD21	1:D:670:LEU:HD12	1.86	0.57
1:A:414:LEU:HD21	1:A:670:LEU:HD12	1.86	0.57
1:B:646:ASP:O	1:B:649:ILE:HG22	2.04	0.57
1:C:386:LEU:HD12	1:C:387:GLY:N	2.19	0.57
1:B:455:ALA:O	1:B:459:GLU:HG2	2.04	0.57
1:C:147:ASN:H	1:C:150:THR:CG2	2.17	0.57
1:C:712:ILE:HD12	1:C:712:ILE:C	2.29	0.57
1:A:499:VAL:HG22	1:A:500:ASP:N	2.18	0.57
1:A:499:VAL:O	1:A:502:HIS:CG	2.56	0.57
1:B:133:PHE:CE1	1:B:198:VAL:HG13	2.39	0.57
1:C:455:ALA:O	1:C:459:GLU:HG2	2.04	0.57
1:B:147:ASN:H	1:B:150:THR:CG2	2.17	0.57
1:A:119:LEU:HD12	1:A:167:VAL:HG11	1.86	0.57
1:A:133:PHE:CE1	1:A:198:VAL:HG13	2.40	0.57
1:A:466:LEU:HD21	1:A:551:VAL:HG21	1.86	0.57
1:C:512:MET:HE2	1:C:512:MET:HA	1.85	0.57
1:D:455:ALA:O	1:D:459:GLU:HG2	2.04	0.57
1:C:133:PHE:CE1	1:C:198:VAL:HG13	2.40	0.57
1:D:386:LEU:HD12	1:D:387:GLY:N	2.19	0.57
1:A:386:LEU:HD12	1:A:387:GLY:N	2.19	0.57
1:A:455:ALA:O	1:A:459:GLU:HG2	2.04	0.57
1:C:77:GLU:O	1:C:80:ASP:HB3	2.04	0.57
1:D:121:LEU:C	1:D:124:PRO:HD2	2.28	0.57
1:D:578:GLY:O	1:D:579:ASP:HB2	2.04	0.57
1:D:133:PHE:CE1	1:D:198:VAL:HG13	2.40	0.57
1:D:229:ARG:HD2	1:D:248:ASP:HB3	1.87	0.57
1:A:229:ARG:HD2	1:A:248:ASP:HB3	1.87	0.56
1:A:488:GLU:HB3	1:A:496:VAL:HG13	1.86	0.56
1:B:414:LEU:HD21	1:B:670:LEU:HD12	1.86	0.56
1:C:414:LEU:HD21	1:C:670:LEU:HD12	1.86	0.56
1:C:447:VAL:CG2	1:C:450:ASN:HB2	2.34	0.56
1:D:99:GLU:HG2	1:D:118:GLN:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:GLU:HB3	1:D:496:VAL:HG13	1.86	0.56
1:B:386:LEU:HD12	1:B:387:GLY:N	2.19	0.56
1:B:499:VAL:H	1:B:502:HIS:HA	1.70	0.56
1:A:99:GLU:HG2	1:A:118:GLN:OE1	2.05	0.56
1:A:121:LEU:C	1:A:124:PRO:HD2	2.29	0.56
1:A:499:VAL:H	1:A:502:HIS:HA	1.70	0.56
1:B:77:GLU:O	1:B:80:ASP:HB3	2.05	0.56
1:B:249:LEU:HB3	1:B:303:VAL:CG2	2.36	0.56
1:B:662:ARG:HA	1:B:662:ARG:HH11	1.70	0.56
1:C:119:LEU:HD12	1:C:167:VAL:HG11	1.86	0.56
1:C:249:LEU:HB3	1:C:303:VAL:CG2	2.36	0.56
1:D:499:VAL:H	1:D:502:HIS:HA	1.70	0.56
1:D:512:MET:HE2	1:D:512:MET:HA	1.87	0.56
1:B:390:THR:O	1:B:394:ILE:HG12	2.06	0.56
1:C:99:GLU:HG2	1:C:118:GLN:OE1	2.06	0.56
1:C:499:VAL:H	1:C:502:HIS:HA	1.71	0.56
1:B:119:LEU:HD12	1:B:167:VAL:HG11	1.86	0.56
1:B:229:ARG:HD2	1:B:248:ASP:HB3	1.87	0.56
1:C:78:TYR:HA	1:C:206:LEU:CD1	2.36	0.56
1:C:229:ARG:HD2	1:C:248:ASP:HB3	1.87	0.56
1:D:539:MET:HE2	1:D:547:ALA:HB3	1.87	0.56
1:C:488:GLU:HB3	1:C:496:VAL:HG13	1.86	0.56
1:A:578:GLY:O	1:A:579:ASP:HB2	2.05	0.56
1:A:662:ARG:HH11	1:A:662:ARG:HA	1.70	0.56
1:B:99:GLU:HG2	1:B:118:GLN:OE1	2.06	0.56
1:B:488:GLU:HB3	1:B:496:VAL:HG13	1.86	0.56
1:C:662:ARG:HA	1:C:662:ARG:HH11	1.70	0.56
1:D:662:ARG:HH11	1:D:662:ARG:HA	1.70	0.56
1:A:77:GLU:O	1:A:80:ASP:HB3	2.05	0.56
1:A:262:GLY:HA2	1:A:305:LYS:O	2.06	0.56
1:A:390:THR:O	1:A:394:ILE:HG12	2.05	0.56
1:B:112:ASN:HA	1:B:116:TRP:CD1	2.41	0.56
1:B:447:VAL:CG2	1:B:450:ASN:HB2	2.35	0.56
1:D:261:ASP:CG	1:D:293:GLY:H	2.14	0.56
1:C:578:GLY:O	1:C:579:ASP:HB2	2.04	0.56
1:D:77:GLU:O	1:D:80:ASP:HB3	2.05	0.56
1:D:657:LEU:O	1:D:658:HIS:HB3	2.06	0.56
1:A:261:ASP:CG	1:A:293:GLY:H	2.14	0.56
1:A:657:LEU:O	1:A:658:HIS:HB3	2.06	0.56
1:B:78:TYR:HA	1:B:206:LEU:CD1	2.36	0.56
1:D:262:GLY:HA2	1:D:305:LYS:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLY:HA3	1:A:103:HIS:O	2.06	0.55
1:A:539:MET:HE2	1:A:547:ALA:HB3	1.88	0.55
1:C:112:ASN:HA	1:C:116:TRP:CD1	2.41	0.55
1:C:638:GLY:O	1:C:652:ALA:HB1	2.06	0.55
1:D:102:GLY:HA3	1:D:103:HIS:O	2.06	0.55
1:A:78:TYR:HA	1:A:206:LEU:CD1	2.35	0.55
1:A:512:MET:HE2	1:A:512:MET:HA	1.89	0.55
1:B:578:GLY:O	1:B:579:ASP:HB2	2.05	0.55
1:D:390:THR:O	1:D:394:ILE:HG12	2.06	0.55
1:A:638:GLY:O	1:A:652:ALA:HB1	2.06	0.55
1:A:125:VAL:O	1:A:129:GLY:HA2	2.07	0.55
1:B:512:MET:HA	1:B:512:MET:HE2	1.88	0.55
1:C:539:MET:HE2	1:C:547:ALA:HB3	1.88	0.55
1:D:260:VAL:HG12	1:D:261:ASP:N	2.22	0.55
1:A:249:LEU:HB3	1:A:303:VAL:CG2	2.36	0.55
1:C:154:MET:O	1:C:158:VAL:HG12	2.07	0.55
1:A:154:MET:O	1:A:158:VAL:HG12	2.07	0.55
1:B:154:MET:O	1:B:158:VAL:HG12	2.07	0.55
1:B:262:GLY:HA2	1:B:305:LYS:O	2.06	0.55
1:C:390:THR:O	1:C:394:ILE:HG12	2.07	0.55
1:C:504:VAL:HB	1:C:541:VAL:HG12	1.89	0.55
1:D:249:LEU:HB3	1:D:303:VAL:CG2	2.36	0.55
1:A:504:VAL:HB	1:A:541:VAL:HG12	1.88	0.55
1:A:575:MET:HE1	1:A:587:VAL:HG13	1.89	0.55
1:B:539:MET:HE2	1:B:547:ALA:HB3	1.88	0.55
1:B:657:LEU:O	1:B:658:HIS:HB3	2.06	0.55
1:C:262:GLY:HA2	1:C:305:LYS:O	2.06	0.55
1:D:229:ARG:HG2	1:D:250:LEU:CD2	2.34	0.55
1:A:260:VAL:HG12	1:A:261:ASP:N	2.22	0.55
1:A:559:THR:HA	1:A:562:THR:HG23	1.89	0.55
1:D:559:THR:HA	1:D:562:THR:HG23	1.89	0.55
1:D:575:MET:HE1	1:D:587:VAL:HG13	1.89	0.55
1:A:229:ARG:HG2	1:A:250:LEU:CD2	2.34	0.55
1:B:504:VAL:HB	1:B:541:VAL:HG12	1.89	0.55
1:C:657:LEU:O	1:C:658:HIS:HB3	2.06	0.55
1:D:112:ASN:HA	1:D:116:TRP:CD1	2.42	0.55
1:D:388:LEU:O	1:D:392:MET:HG3	2.07	0.55
1:B:638:GLY:O	1:B:652:ALA:HB1	2.07	0.54
1:D:310:GLY:O	1:D:313:THR:HG22	2.07	0.54
1:D:504:VAL:HB	1:D:541:VAL:HG12	1.89	0.54
1:A:310:GLY:O	1:A:313:THR:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:TRP:CE3	1:B:369:TYR:HB3	2.42	0.54
1:C:270:PHE:CD1	1:C:282:PRO:HB2	2.42	0.54
1:B:261:ASP:CG	1:B:293:GLY:H	2.14	0.54
1:B:270:PHE:CD1	1:B:282:PRO:HB2	2.42	0.54
1:B:718:ALA:O	1:B:722:VAL:HG12	2.06	0.54
1:D:154:MET:O	1:D:158:VAL:HG12	2.07	0.54
1:B:502:HIS:CE1	1:C:520:ALA:HA	2.42	0.54
1:C:358:TRP:CE3	1:C:369:TYR:HB3	2.43	0.54
1:C:735:THR:O	1:C:736:LEU:C	2.51	0.54
1:D:78:TYR:HA	1:D:206:LEU:CD1	2.37	0.54
1:A:388:LEU:O	1:A:392:MET:HG3	2.08	0.54
1:B:110:SER:O	1:B:111:GLY:C	2.51	0.54
1:B:735:THR:O	1:B:736:LEU:C	2.51	0.54
1:C:85:PHE:CZ	1:C:200:LEU:HD13	2.43	0.54
1:C:261:ASP:CG	1:C:293:GLY:H	2.14	0.54
1:C:310:GLY:O	1:C:313:THR:HG22	2.07	0.54
1:D:718:ALA:O	1:D:722:VAL:HG12	2.07	0.54
1:A:112:ASN:HA	1:A:116:TRP:CD1	2.43	0.54
1:B:102:GLY:HA3	1:B:103:HIS:O	2.06	0.54
1:C:718:ALA:O	1:C:722:VAL:HG12	2.07	0.54
1:D:125:VAL:O	1:D:129:GLY:HA2	2.08	0.54
1:D:638:GLY:O	1:D:652:ALA:HB1	2.07	0.54
1:A:229:ARG:NH1	1:A:239:VAL:HG21	2.22	0.54
1:B:310:GLY:O	1:B:313:THR:HG22	2.07	0.54
1:C:102:GLY:HA3	1:C:103:HIS:O	2.06	0.54
1:A:358:TRP:CE3	1:A:369:TYR:HB3	2.42	0.54
1:B:388:LEU:O	1:B:392:MET:HG3	2.07	0.54
1:B:693:VAL:HG22	1:B:694:PRO:HD3	1.90	0.54
1:C:110:SER:O	1:C:111:GLY:C	2.51	0.54
1:C:260:VAL:HG12	1:C:261:ASP:N	2.21	0.54
1:D:229:ARG:NH1	1:D:239:VAL:HG21	2.22	0.54
1:A:504:VAL:HA	1:A:540:ALA:O	2.08	0.54
1:C:606:SER:HB2	1:C:630:PRO:HB2	1.90	0.54
1:C:214:SER:HB2	1:C:217:ARG:HG2	1.89	0.54
1:C:709:SER:OG	1:C:712:ILE:HG23	2.08	0.54
1:D:126:VAL:HG21	1:D:191:ALA:HB1	1.90	0.54
1:D:342:TRP:C	1:D:345:PRO:HD2	2.33	0.54
1:D:358:TRP:CE3	1:D:369:TYR:HB3	2.43	0.54
1:A:735:THR:O	1:A:736:LEU:C	2.51	0.53
1:B:260:VAL:HG12	1:B:261:ASP:N	2.22	0.53
1:B:559:THR:HA	1:B:562:THR:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:GLU:CG	1:C:233:ASP:N	2.70	0.53
1:D:735:THR:O	1:D:736:LEU:C	2.51	0.53
1:A:85:PHE:CZ	1:A:200:LEU:HD13	2.43	0.53
1:A:126:VAL:HG21	1:A:191:ALA:HB1	1.90	0.53
1:A:541:VAL:HG13	1:A:546:VAL:HG21	1.90	0.53
1:B:214:SER:HB2	1:B:217:ARG:HG2	1.89	0.53
1:B:232:GLU:CG	1:B:233:ASP:N	2.70	0.53
1:B:600:ILE:HB	1:B:604:ASP:OD1	2.09	0.53
1:C:559:THR:HA	1:C:562:THR:HG23	1.89	0.53
1:D:504:VAL:HA	1:D:540:ALA:O	2.08	0.53
1:D:541:VAL:HG13	1:D:546:VAL:HG21	1.90	0.53
1:A:132:PRO:O	1:A:136:ARG:HG3	2.09	0.53
1:A:270:PHE:CD1	1:A:282:PRO:HB2	2.42	0.53
1:A:342:TRP:C	1:A:345:PRO:HD2	2.34	0.53
1:A:613:LYS:HE2	1:A:636:ASP:OD1	2.09	0.53
1:B:85:PHE:CZ	1:B:200:LEU:HD13	2.43	0.53
1:B:606:SER:HB2	1:B:630:PRO:HB2	1.91	0.53
1:C:388:LEU:O	1:C:392:MET:HG3	2.08	0.53
1:C:600:ILE:HB	1:C:604:ASP:OD1	2.09	0.53
1:D:270:PHE:CD1	1:D:282:PRO:HB2	2.42	0.53
1:A:482:GLY:HA3	1:A:499:VAL:CG2	2.35	0.53
1:B:229:ARG:NH1	1:B:239:VAL:HG21	2.22	0.53
1:D:600:ILE:HB	1:D:604:ASP:OD1	2.09	0.53
1:A:160:TRP:O	1:A:164:MET:CB	2.56	0.53
1:A:227:ALA:HB1	1:A:250:LEU:HD11	1.90	0.53
1:C:229:ARG:NH1	1:C:239:VAL:HG21	2.22	0.53
1:C:342:TRP:C	1:C:345:PRO:HD2	2.33	0.53
1:D:160:TRP:O	1:D:164:MET:CB	2.56	0.53
1:D:227:ALA:HB1	1:D:250:LEU:HD11	1.90	0.53
1:A:600:ILE:HB	1:A:604:ASP:OD1	2.09	0.53
1:C:575:MET:HE1	1:C:587:VAL:HG13	1.91	0.53
1:D:110:SER:O	1:D:111:GLY:C	2.50	0.53
1:D:214:SER:HB2	1:D:217:ARG:HG2	1.89	0.53
1:D:709:SER:OG	1:D:712:ILE:HG23	2.08	0.53
1:A:214:SER:HB2	1:A:217:ARG:HG2	1.89	0.53
1:A:499:VAL:O	1:A:502:HIS:HA	2.08	0.53
1:B:660:ASP:O	1:B:662:ARG:HG2	2.09	0.53
1:C:229:ARG:HG2	1:C:250:LEU:CD2	2.34	0.53
1:D:166:ALA:HA	1:D:173:PHE:CE2	2.44	0.53
1:D:499:VAL:O	1:D:502:HIS:HA	2.08	0.53
1:A:166:ALA:HA	1:A:173:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:SER:O	1:A:285:LYS:HB2	2.09	0.53
1:B:229:ARG:HG2	1:B:250:LEU:CD2	2.34	0.53
1:B:575:MET:HE1	1:B:587:VAL:HG13	1.91	0.53
1:C:166:ALA:HA	1:C:173:PHE:CE2	2.44	0.53
1:D:482:GLY:HA3	1:D:499:VAL:CG2	2.36	0.53
1:D:613:LYS:HE2	1:D:636:ASP:OD1	2.09	0.53
1:A:555:ILE:HD12	1:A:555:ILE:O	2.09	0.53
1:A:693:VAL:HG22	1:A:694:PRO:HD3	1.90	0.53
1:B:499:VAL:O	1:B:502:HIS:HA	2.09	0.53
1:C:499:VAL:O	1:C:502:HIS:HA	2.09	0.53
1:C:693:VAL:HG22	1:C:694:PRO:HD3	1.91	0.53
1:D:693:VAL:HG22	1:D:694:PRO:HD3	1.90	0.53
1:B:342:TRP:C	1:B:345:PRO:HD2	2.34	0.53
1:B:482:GLY:HA3	1:B:499:VAL:CG2	2.35	0.53
1:B:504:VAL:HA	1:B:540:ALA:O	2.09	0.53
1:B:604:ASP:HB3	1:B:607:ARG:NH2	2.25	0.53
1:B:709:SER:OG	1:B:712:ILE:HG23	2.09	0.53
1:C:482:GLY:HA3	1:C:499:VAL:CG2	2.35	0.53
1:D:132:PRO:O	1:D:136:ARG:HG3	2.09	0.53
1:A:110:SER:O	1:A:111:GLY:C	2.51	0.52
1:A:660:ASP:O	1:A:662:ARG:HG2	2.09	0.52
1:A:718:ALA:O	1:A:722:VAL:HG12	2.09	0.52
1:B:613:LYS:HE2	1:B:636:ASP:OD1	2.09	0.52
1:C:613:LYS:HE2	1:C:636:ASP:OD1	2.09	0.52
1:D:179:SER:HB3	1:D:181:GLU:C	2.34	0.52
1:D:269:SER:O	1:D:285:LYS:HB2	2.09	0.52
1:B:166:ALA:HA	1:B:173:PHE:CE2	2.44	0.52
1:B:541:VAL:HG13	1:B:546:VAL:HG21	1.90	0.52
1:B:702:PRO:O	1:B:703:LEU:C	2.52	0.52
1:C:604:ASP:HB3	1:C:607:ARG:NH2	2.25	0.52
1:D:85:PHE:CZ	1:D:200:LEU:HD13	2.44	0.52
1:D:391:PRO:O	1:D:395:MET:HG2	2.08	0.52
1:D:604:ASP:HB3	1:D:607:ARG:NH2	2.25	0.52
1:D:660:ASP:O	1:D:662:ARG:HG2	2.09	0.52
1:A:340:SER:O	1:A:344:VAL:HG13	2.09	0.52
1:A:604:ASP:HB3	1:A:607:ARG:NH2	2.25	0.52
1:A:391:PRO:O	1:A:395:MET:HG2	2.09	0.52
1:B:446:PHE:HE2	1:B:451:ALA:HB2	1.75	0.52
1:C:504:VAL:HA	1:C:540:ALA:O	2.09	0.52
1:D:555:ILE:O	1:D:555:ILE:HD12	2.09	0.52
1:D:606:SER:HB2	1:D:630:PRO:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD12	1:A:106:LYS:H	1.73	0.52
1:B:227:ALA:HB1	1:B:250:LEU:HD11	1.90	0.52
1:C:125:VAL:O	1:C:129:GLY:HA2	2.08	0.52
1:C:541:VAL:HG13	1:C:546:VAL:HG21	1.90	0.52
1:C:660:ASP:O	1:C:662:ARG:HG2	2.10	0.52
1:C:702:PRO:O	1:C:703:LEU:C	2.52	0.52
1:D:340:SER:O	1:D:344:VAL:HG13	2.10	0.52
1:A:474:ALA:O	1:A:478:GLY:N	2.42	0.52
1:A:606:SER:HB2	1:A:630:PRO:HB2	1.91	0.52
1:C:227:ALA:HB1	1:C:250:LEU:HD11	1.90	0.52
1:D:105:LEU:HD12	1:D:106:LYS:H	1.73	0.52
1:A:266:GLU:N	1:A:303:VAL:HG12	2.25	0.52
1:B:132:PRO:O	1:B:136:ARG:HG3	2.09	0.52
1:D:474:ALA:O	1:D:478:GLY:N	2.42	0.52
1:A:705:GLY:O	1:A:706:LEU:HG	2.09	0.52
1:B:266:GLU:N	1:B:303:VAL:HG12	2.25	0.52
1:C:266:GLU:N	1:C:303:VAL:HG12	2.25	0.52
1:C:340:SER:O	1:C:344:VAL:HG13	2.10	0.52
1:D:266:GLU:N	1:D:303:VAL:HG12	2.25	0.52
1:D:616:GLY:C	1:D:617:LEU:HD12	2.35	0.52
1:A:78:TYR:HA	1:A:206:LEU:HD12	1.92	0.52
1:A:419:LYS:C	1:A:618:ILE:HD12	2.34	0.52
1:A:616:GLY:C	1:A:617:LEU:HD12	2.35	0.52
1:B:82:ARG:O	1:B:86:TRP:HD1	1.93	0.52
1:B:125:VAL:O	1:B:129:GLY:HA2	2.09	0.52
1:B:555:ILE:O	1:B:555:ILE:HD12	2.09	0.52
1:C:269:SER:O	1:C:285:LYS:HB2	2.09	0.52
1:C:446:PHE:HE2	1:C:451:ALA:HB2	1.75	0.52
1:A:510:ARG:HG3	1:A:514:GLU:OE1	2.10	0.52
1:B:105:LEU:HD12	1:B:106:LYS:H	1.73	0.52
1:B:450:ASN:HD22	1:C:513:GLN:HG3	1.75	0.52
1:B:510:ARG:HG3	1:B:514:GLU:OE1	2.10	0.52
1:B:616:GLY:C	1:B:617:LEU:HD12	2.35	0.52
1:C:82:ARG:O	1:C:86:TRP:HD1	1.93	0.52
1:C:160:TRP:O	1:C:164:MET:CB	2.57	0.52
1:D:78:TYR:HA	1:D:206:LEU:HD12	1.92	0.52
1:D:705:GLY:O	1:D:706:LEU:HG	2.09	0.52
1:A:179:SER:HB3	1:A:181:GLU:C	2.36	0.51
1:A:709:SER:OG	1:A:712:ILE:HG23	2.10	0.51
1:B:269:SER:O	1:B:285:LYS:HB2	2.09	0.51
1:B:340:SER:O	1:B:344:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:PRO:O	1:B:395:MET:HG2	2.09	0.51
1:B:440:ARG:HB3	1:B:550:VAL:CG2	2.40	0.51
1:C:391:PRO:O	1:C:395:MET:HG2	2.08	0.51
1:C:440:ARG:HB3	1:C:550:VAL:CG2	2.40	0.51
1:C:474:ALA:O	1:C:478:GLY:N	2.42	0.51
1:C:555:ILE:HD12	1:C:555:ILE:O	2.09	0.51
1:C:616:GLY:C	1:C:617:LEU:HD12	2.35	0.51
1:B:179:SER:HB3	1:B:181:GLU:C	2.35	0.51
1:B:474:ALA:O	1:B:478:GLY:N	2.42	0.51
1:B:479:LEU:C	1:B:479:LEU:HD22	2.35	0.51
1:D:131:TRP:HB3	1:D:132:PRO:HD3	1.92	0.51
1:D:510:ARG:HG3	1:D:514:GLU:OE1	2.10	0.51
1:A:446:PHE:HE2	1:A:451:ALA:HB2	1.74	0.51
1:B:363:PRO:HB2	1:B:364:GLN:NE2	2.26	0.51
1:C:105:LEU:HD12	1:C:106:LYS:H	1.73	0.51
1:C:132:PRO:O	1:C:136:ARG:HG3	2.09	0.51
1:C:363:PRO:HB2	1:C:364:GLN:NE2	2.26	0.51
1:C:419:LYS:C	1:C:618:ILE:HD12	2.35	0.51
1:C:479:LEU:C	1:C:479:LEU:HD22	2.35	0.51
1:A:376:SER:HA	1:A:379:ILE:HG22	1.93	0.51
1:B:160:TRP:O	1:B:164:MET:CB	2.57	0.51
1:C:179:SER:HB3	1:C:181:GLU:C	2.35	0.51
1:D:363:PRO:HB2	1:D:364:GLN:NE2	2.26	0.51
1:A:363:PRO:HB2	1:A:364:GLN:NE2	2.26	0.51
1:A:702:PRO:O	1:A:703:LEU:C	2.52	0.51
1:C:216:ILE:HG21	1:C:326:GLN:NE2	2.26	0.51
1:C:510:ARG:HG3	1:C:514:GLU:OE1	2.10	0.51
1:D:702:PRO:O	1:D:703:LEU:C	2.52	0.51
1:B:417:MET:HE1	1:B:639:ILE:HD11	1.93	0.51
1:B:705:GLY:O	1:B:706:LEU:HG	2.10	0.51
1:C:376:SER:HA	1:C:379:ILE:HG22	1.93	0.51
1:C:705:GLY:O	1:C:706:LEU:HG	2.10	0.51
1:D:417:MET:HE1	1:D:639:ILE:HD11	1.92	0.51
1:D:446:PHE:HE2	1:D:451:ALA:HB2	1.75	0.51
1:A:440:ARG:HB3	1:A:550:VAL:CG2	2.40	0.51
1:B:216:ILE:HG21	1:B:326:GLN:NE2	2.26	0.51
1:B:376:SER:HA	1:B:379:ILE:HG22	1.93	0.51
1:B:419:LYS:C	1:B:618:ILE:HD12	2.35	0.51
1:B:425:VAL:HG12	1:B:622:ALA:HB3	1.93	0.51
1:C:425:VAL:HG12	1:C:622:ALA:HB3	1.93	0.51
1:D:440:ARG:HB3	1:D:550:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ARG:O	1:D:86:TRP:HD1	1.93	0.51
1:A:82:ARG:O	1:A:86:TRP:HD1	1.93	0.51
1:C:417:MET:HE1	1:C:639:ILE:HD11	1.93	0.51
1:D:376:SER:HA	1:D:379:ILE:HG22	1.93	0.51
1:D:417:MET:HG3	1:D:668:ARG:HA	1.93	0.51
1:D:419:LYS:C	1:D:618:ILE:HD12	2.35	0.51
1:A:417:MET:HG3	1:A:668:ARG:HA	1.93	0.50
1:A:536:VAL:HG13	1:A:550:VAL:HG12	1.93	0.50
1:D:479:LEU:C	1:D:479:LEU:HD22	2.35	0.50
1:A:75:SER:HB3	1:A:78:TYR:HB3	1.93	0.50
1:A:131:TRP:HB3	1:A:132:PRO:HD3	1.93	0.50
1:A:163:SER:OG	1:A:186:VAL:HG23	2.11	0.50
1:A:219:LEU:C	1:A:219:LEU:HD22	2.36	0.50
1:A:479:LEU:C	1:A:479:LEU:HD22	2.35	0.50
1:B:447:VAL:HG13	1:C:510:ARG:HH12	1.76	0.50
1:C:126:VAL:HG21	1:C:191:ALA:HB1	1.91	0.50
1:A:428:THR:O	2:A:995:ALF:F2	2.19	0.50
1:B:616:GLY:O	1:B:617:LEU:HD12	2.12	0.50
1:C:358:TRP:O	1:C:362:GLY:HA3	2.11	0.50
1:D:219:LEU:C	1:D:219:LEU:HD22	2.36	0.50
1:A:216:ILE:HG21	1:A:326:GLN:NE2	2.26	0.50
1:B:163:SER:OG	1:B:186:VAL:HG23	2.12	0.50
1:B:365:PRO:HA	1:B:366:ALA:C	2.37	0.50
1:C:179:SER:N	1:C:180:GLN:HA	2.27	0.50
1:C:308:HIS:HB3	1:C:312:ASP:OD1	2.12	0.50
1:C:616:GLY:O	1:C:617:LEU:HD12	2.12	0.50
1:C:695:LEU:HD12	1:C:695:LEU:C	2.37	0.50
1:D:216:ILE:HG21	1:D:326:GLN:NE2	2.26	0.50
1:D:616:GLY:O	1:D:617:LEU:HD12	2.12	0.50
1:A:219:LEU:CD2	1:A:647:VAL:HG12	2.42	0.50
1:B:358:TRP:O	1:B:362:GLY:HA3	2.12	0.50
1:B:605:LYS:HD3	1:B:628:ASP:HB3	1.93	0.50
1:B:695:LEU:C	1:B:695:LEU:HD12	2.37	0.50
1:D:219:LEU:CD2	1:D:647:VAL:HG12	2.42	0.50
1:D:605:LYS:HD3	1:D:628:ASP:HB3	1.93	0.50
1:A:417:MET:HE1	1:A:639:ILE:HD11	1.93	0.50
1:A:616:GLY:O	1:A:617:LEU:HD12	2.12	0.50
1:B:75:SER:HB3	1:B:78:TYR:HB3	1.93	0.50
1:B:308:HIS:HB3	1:B:312:ASP:OD1	2.12	0.50
1:C:131:TRP:HB3	1:C:132:PRO:HD3	1.93	0.50
1:C:414:LEU:HD21	1:C:670:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:MET:HG3	1:C:668:ARG:HA	1.93	0.50
1:A:358:TRP:O	1:A:362:GLY:HA3	2.11	0.50
1:B:131:TRP:HB3	1:B:132:PRO:HD3	1.93	0.50
1:B:179:SER:N	1:B:180:GLN:HA	2.27	0.50
1:C:163:SER:OG	1:C:186:VAL:HG23	2.12	0.50
1:C:365:PRO:HA	1:C:366:ALA:C	2.37	0.50
1:D:75:SER:HB3	1:D:78:TYR:HB3	1.93	0.50
1:B:417:MET:HG3	1:B:668:ARG:HA	1.93	0.50
1:C:75:SER:HB3	1:C:78:TYR:HB3	1.93	0.50
1:C:258:ILE:HD12	1:C:295:THR:CG2	2.42	0.50
1:D:163:SER:OG	1:D:186:VAL:HG23	2.12	0.50
1:D:358:TRP:O	1:D:362:GLY:HA3	2.11	0.50
1:D:657:LEU:C	1:D:659:GLY:HA2	2.37	0.50
1:A:367:LEU:CD1	1:A:367:LEU:H	2.25	0.50
1:B:219:LEU:C	1:B:219:LEU:HD22	2.36	0.50
1:B:266:GLU:H	1:B:303:VAL:HG12	1.77	0.50
1:B:414:LEU:HD21	1:B:670:LEU:CD1	2.42	0.50
1:C:219:LEU:HD22	1:C:219:LEU:C	2.36	0.50
1:D:232:GLU:CG	1:D:233:ASP:N	2.70	0.50
1:D:425:VAL:HG12	1:D:622:ALA:HB3	1.93	0.50
1:A:232:GLU:CG	1:A:233:ASP:N	2.70	0.49
1:A:657:LEU:HG	1:A:658:HIS:N	2.27	0.49
1:A:657:LEU:C	1:A:659:GLY:HA2	2.37	0.49
1:B:90:MET:O	1:B:94:PRO:HD3	2.12	0.49
1:B:657:LEU:C	1:B:659:GLY:HA2	2.37	0.49
1:D:695:LEU:C	1:D:695:LEU:HD12	2.37	0.49
1:B:78:TYR:HA	1:B:206:LEU:HD12	1.93	0.49
1:C:266:GLU:H	1:C:303:VAL:HG12	1.77	0.49
1:C:657:LEU:C	1:C:659:GLY:HA2	2.37	0.49
1:C:688:TYR:CE1	1:C:719:LEU:HD23	2.47	0.49
1:D:615:LYS:HG3	1:D:616:GLY:N	2.25	0.49
1:A:86:TRP:HB2	1:C:703:LEU:HD21	1.93	0.49
1:A:605:LYS:HD3	1:A:628:ASP:HB3	1.94	0.49
1:A:615:LYS:HG3	1:A:616:GLY:N	2.26	0.49
1:A:695:LEU:HD12	1:A:695:LEU:C	2.37	0.49
1:B:126:VAL:HG21	1:B:191:ALA:HB1	1.93	0.49
1:B:260:VAL:CG1	1:B:261:ASP:N	2.75	0.49
1:B:680:GLN:O	1:B:683:PHE:HB3	2.12	0.49
1:C:78:TYR:HA	1:C:206:LEU:HD12	1.93	0.49
1:C:260:VAL:CG1	1:C:261:ASP:N	2.75	0.49
1:C:276:VAL:HG13	1:C:602:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ILE:HD12	1:D:295:THR:CG2	2.42	0.49
1:D:367:LEU:CD1	1:D:367:LEU:H	2.26	0.49
1:D:687:ILE:HA	1:D:690:VAL:CG1	2.41	0.49
1:A:276:VAL:HG13	1:A:602:PRO:HD3	1.94	0.49
1:A:365:PRO:HA	1:A:366:ALA:C	2.37	0.49
1:A:425:VAL:HG12	1:A:622:ALA:HB3	1.94	0.49
1:A:468:ASN:HA	1:A:471:VAL:HG22	1.94	0.49
1:C:605:LYS:HD3	1:C:628:ASP:HB3	1.94	0.49
1:D:260:VAL:CG1	1:D:261:ASP:N	2.75	0.49
1:D:468:ASN:HA	1:D:471:VAL:HG22	1.94	0.49
1:D:536:VAL:HG13	1:D:550:VAL:HG12	1.95	0.49
1:D:657:LEU:HG	1:D:658:HIS:N	2.27	0.49
1:A:260:VAL:CG1	1:A:261:ASP:N	2.75	0.49
1:C:90:MET:O	1:C:94:PRO:HD3	2.13	0.49
1:C:258:ILE:HD12	1:C:295:THR:HG23	1.95	0.49
1:D:276:VAL:HG13	1:D:602:PRO:HD3	1.94	0.49
1:A:308:HIS:HB3	1:A:312:ASP:OD1	2.12	0.49
1:B:162:TYR:HB2	1:B:375:VAL:HG11	1.94	0.49
1:B:219:LEU:CD2	1:B:647:VAL:HG12	2.42	0.49
1:B:258:ILE:HD12	1:B:295:THR:CG2	2.43	0.49
1:D:159:ALA:CB	1:D:379:ILE:HD13	2.41	0.49
1:D:365:PRO:HA	1:D:366:ALA:C	2.37	0.49
1:D:414:LEU:HD21	1:D:670:LEU:CD1	2.42	0.49
1:A:179:SER:N	1:A:180:GLN:HA	2.27	0.49
1:A:258:ILE:HD12	1:A:295:THR:CG2	2.43	0.49
1:A:266:GLU:H	1:A:303:VAL:HG12	1.77	0.49
1:A:414:LEU:HD21	1:A:670:LEU:CD1	2.42	0.49
1:B:276:VAL:HG13	1:B:602:PRO:HD3	1.94	0.49
1:B:687:ILE:HA	1:B:690:VAL:CG1	2.42	0.49
1:C:219:LEU:CD2	1:C:647:VAL:HG12	2.42	0.49
1:C:693:VAL:N	1:C:694:PRO:HD2	2.28	0.49
1:D:308:HIS:HB3	1:D:312:ASP:OD1	2.12	0.49
1:D:680:GLN:O	1:D:683:PHE:HB3	2.12	0.49
1:B:152:ILE:O	1:B:156:ILE:HG12	2.13	0.49
1:B:163:SER:O	1:B:167:VAL:HG12	2.13	0.49
1:B:468:ASN:HA	1:B:471:VAL:HG22	1.94	0.49
1:B:703:LEU:HD21	1:D:86:TRP:HB2	1.95	0.49
1:D:179:SER:N	1:D:180:GLN:HA	2.27	0.49
1:A:78:TYR:CD2	1:A:79:LEU:HD12	2.42	0.49
1:A:152:ILE:O	1:A:156:ILE:HG12	2.13	0.49
1:B:367:LEU:H	1:B:367:LEU:CD1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:VAL:N	1:B:694:PRO:HD2	2.28	0.49
1:C:468:ASN:HA	1:C:471:VAL:HG22	1.94	0.49
1:D:152:ILE:O	1:D:156:ILE:HG12	2.13	0.49
1:D:266:GLU:H	1:D:303:VAL:HG12	1.77	0.49
1:B:605:LYS:CD	1:B:628:ASP:HB3	2.43	0.49
1:B:657:LEU:HG	1:B:658:HIS:N	2.27	0.49
1:C:152:ILE:O	1:C:156:ILE:HG12	2.13	0.49
1:C:657:LEU:HG	1:C:658:HIS:N	2.27	0.49
1:A:220:LEU:HG	1:A:647:VAL:HG11	1.96	0.48
1:A:680:GLN:O	1:A:683:PHE:HB3	2.13	0.48
1:B:447:VAL:HG22	1:C:513:GLN:OE1	2.12	0.48
1:C:367:LEU:H	1:C:367:LEU:CD1	2.25	0.48
1:C:536:VAL:HG13	1:C:550:VAL:HG12	1.95	0.48
1:C:687:ILE:HA	1:C:690:VAL:CG1	2.42	0.48
1:A:90:MET:O	1:A:94:PRO:HD3	2.13	0.48
1:A:687:ILE:HA	1:A:690:VAL:CG1	2.42	0.48
1:A:688:TYR:CE1	1:A:719:LEU:HD23	2.47	0.48
1:D:430:THR:HG22	1:D:641:MET:HG3	1.94	0.48
1:D:605:LYS:CD	1:D:628:ASP:HB3	2.43	0.48
1:A:426:ASP:OD2	2:A:995:ALF:F2	2.20	0.48
1:B:258:ILE:HD12	1:B:295:THR:HG23	1.95	0.48
1:B:639:ILE:CG2	1:B:656:LEU:HD13	2.43	0.48
1:D:90:MET:O	1:D:94:PRO:HD3	2.13	0.48
1:D:162:TYR:HB2	1:D:375:VAL:HG11	1.95	0.48
1:D:220:LEU:HG	1:D:647:VAL:HG11	1.96	0.48
1:A:269:SER:HB3	1:A:300:GLY:HA3	1.96	0.48
1:B:143:THR:OG1	1:B:144:GLY:N	2.47	0.48
1:C:639:ILE:CG2	1:C:656:LEU:HD13	2.43	0.48
1:C:680:GLN:O	1:C:683:PHE:HB3	2.13	0.48
1:D:78:TYR:CD2	1:D:79:LEU:HD12	2.43	0.48
1:A:162:TYR:HB2	1:A:375:VAL:HG11	1.95	0.48
1:A:163:SER:O	1:A:167:VAL:HG12	2.13	0.48
1:A:510:ARG:O	1:A:514:GLU:HG3	2.13	0.48
1:A:143:THR:OG1	1:A:144:GLY:N	2.47	0.48
1:A:605:LYS:CD	1:A:628:ASP:HB3	2.44	0.48
1:B:220:LEU:HG	1:B:647:VAL:HG11	1.95	0.48
1:B:224:PRO:O	1:B:241:LEU:HD22	2.14	0.48
1:B:510:ARG:O	1:B:514:GLU:HG3	2.13	0.48
1:C:143:THR:OG1	1:C:144:GLY:N	2.47	0.48
1:C:162:TYR:HB2	1:C:375:VAL:HG11	1.95	0.48
1:C:224:PRO:O	1:C:241:LEU:HD22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:THR:OG1	1:D:144:GLY:N	2.47	0.48
1:D:269:SER:HB3	1:D:300:GLY:HA3	1.96	0.48
1:D:510:ARG:O	1:D:514:GLU:HG3	2.13	0.48
1:B:536:VAL:HG13	1:B:550:VAL:HG12	1.96	0.48
1:C:220:LEU:HG	1:C:647:VAL:HG11	1.96	0.48
1:C:636:ASP:O	1:C:637:ILE:HD13	2.14	0.48
1:C:657:LEU:O	1:C:658:HIS:CB	2.61	0.48
1:D:390:THR:N	1:D:391:PRO:HD2	2.29	0.48
1:D:693:VAL:N	1:D:694:PRO:HD2	2.29	0.48
1:A:224:PRO:O	1:A:241:LEU:HD22	2.14	0.48
1:B:440:ARG:HB3	1:B:550:VAL:HG21	1.96	0.48
1:B:544:LYS:O	1:B:546:VAL:HG13	2.14	0.48
1:B:657:LEU:O	1:B:658:HIS:CB	2.61	0.48
1:C:163:SER:O	1:C:167:VAL:HG12	2.14	0.48
1:D:163:SER:O	1:D:167:VAL:HG12	2.14	0.48
1:D:692:GLY:O	1:D:695:LEU:HG	2.14	0.48
1:C:605:LYS:CD	1:C:628:ASP:HB3	2.44	0.48
1:D:119:LEU:HD23	1:D:119:LEU:C	2.39	0.48
1:D:136:ARG:HD2	1:D:149:PHE:CE2	2.49	0.48
1:A:159:ALA:CB	1:A:379:ILE:HD13	2.42	0.48
1:A:390:THR:N	1:A:391:PRO:HD2	2.29	0.48
1:B:636:ASP:O	1:B:637:ILE:HD13	2.14	0.48
1:C:119:LEU:C	1:C:119:LEU:HD23	2.38	0.48
1:C:510:ARG:O	1:C:514:GLU:HG3	2.13	0.48
1:A:657:LEU:O	1:A:658:HIS:CB	2.61	0.47
1:A:671:SER:O	1:A:672:GLU:C	2.57	0.47
1:A:693:VAL:N	1:A:694:PRO:HD2	2.29	0.47
1:C:269:SER:HB3	1:C:300:GLY:HA3	1.96	0.47
1:D:657:LEU:O	1:D:658:HIS:CB	2.61	0.47
1:A:636:ASP:O	1:A:637:ILE:HD13	2.14	0.47
1:B:269:SER:HB3	1:B:300:GLY:HA3	1.96	0.47
1:B:688:TYR:CE1	1:B:719:LEU:HD23	2.49	0.47
1:C:430:THR:HG22	1:C:641:MET:HG3	1.95	0.47
1:C:440:ARG:HB3	1:C:550:VAL:HG21	1.97	0.47
1:D:224:PRO:O	1:D:241:LEU:HD22	2.14	0.47
1:D:440:ARG:HB3	1:D:550:VAL:HG21	1.96	0.47
1:D:671:SER:O	1:D:672:GLU:C	2.57	0.47
1:A:119:LEU:C	1:A:119:LEU:HD23	2.40	0.47
1:A:136:ARG:HD2	1:A:149:PHE:CE2	2.50	0.47
1:A:440:ARG:HB3	1:A:550:VAL:HG21	1.96	0.47
1:A:692:GLY:O	1:A:695:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ASN:O	1:C:298:GLN:HG3	2.14	0.47
1:D:233:ASP:C	1:D:235:SER:H	2.23	0.47
1:A:233:ASP:C	1:A:235:SER:H	2.23	0.47
1:C:146:LEU:HD13	1:C:344:VAL:HG22	1.97	0.47
1:C:692:GLY:O	1:C:695:LEU:HG	2.14	0.47
1:D:92:THR:O	1:D:95:VAL:HB	2.15	0.47
1:D:258:ILE:HD12	1:D:295:THR:HG23	1.96	0.47
1:A:146:LEU:HD13	1:A:344:VAL:HG22	1.97	0.47
1:A:216:ILE:HG21	1:A:326:GLN:HE22	1.79	0.47
1:A:258:ILE:HD12	1:A:295:THR:HG23	1.96	0.47
1:A:430:THR:HG22	1:A:641:MET:HG3	1.95	0.47
1:B:297:ASN:O	1:B:298:GLN:HG3	2.14	0.47
1:B:692:GLY:O	1:B:695:LEU:HG	2.15	0.47
1:C:216:ILE:HD11	1:C:322:VAL:HG21	1.97	0.47
1:D:224:PRO:HD3	1:D:257:LYS:HD2	1.97	0.47
1:A:224:PRO:HD3	1:A:257:LYS:HD2	1.97	0.47
1:B:159:ALA:CB	1:B:379:ILE:HD13	2.41	0.47
1:B:224:PRO:HD3	1:B:257:LYS:HD2	1.97	0.47
1:B:708:LEU:HD13	1:B:709:SER:N	2.30	0.47
1:C:224:PRO:HD3	1:C:257:LYS:HD2	1.97	0.47
1:A:539:MET:CE	1:A:547:ALA:HB3	2.45	0.47
1:B:216:ILE:HD11	1:B:322:VAL:HG21	1.97	0.47
1:B:367:LEU:C	1:B:367:LEU:HD22	2.40	0.47
1:B:430:THR:HG22	1:B:641:MET:HG3	1.95	0.47
1:B:615:LYS:HG3	1:B:616:GLY:N	2.25	0.47
1:B:657:LEU:O	1:B:659:GLY:HA2	2.14	0.47
1:C:367:LEU:C	1:C:367:LEU:HD22	2.40	0.47
1:C:615:LYS:HG3	1:C:616:GLY:N	2.25	0.47
1:C:708:LEU:HD13	1:C:709:SER:N	2.30	0.47
1:D:131:TRP:N	1:D:132:PRO:CD	2.77	0.47
1:D:216:ILE:HG21	1:D:326:GLN:HE22	1.79	0.47
1:D:636:ASP:O	1:D:637:ILE:HD13	2.15	0.47
1:A:92:THR:O	1:A:95:VAL:HB	2.15	0.47
1:A:297:ASN:O	1:A:298:GLN:HG3	2.14	0.47
1:B:119:LEU:HD23	1:B:119:LEU:C	2.39	0.47
1:C:657:LEU:O	1:C:659:GLY:HA2	2.14	0.47
1:D:297:ASN:O	1:D:298:GLN:HG3	2.14	0.47
1:D:407:LEU:N	1:D:407:LEU:HD23	2.28	0.47
1:D:605:LYS:CE	1:D:628:ASP:HB3	2.44	0.47
1:D:713:ALA:O	1:D:717:MET:HG3	2.15	0.47
1:A:690:VAL:HA	1:A:693:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLY:CA	1:B:103:HIS:C	2.77	0.47
1:B:233:ASP:C	1:B:235:SER:H	2.23	0.47
1:C:92:THR:O	1:C:95:VAL:HB	2.15	0.47
1:D:216:ILE:HD11	1:D:322:VAL:HG21	1.97	0.47
1:D:539:MET:CE	1:D:547:ALA:HB3	2.45	0.47
1:D:540:ALA:HB2	1:D:545:THR:HA	1.97	0.47
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.74	0.47
1:A:605:LYS:CE	1:A:628:ASP:HB3	2.44	0.47
1:B:146:LEU:HD13	1:B:344:VAL:HG22	1.97	0.47
1:B:179:SER:CB	1:B:183:VAL:HG22	2.45	0.47
1:B:308:HIS:HB3	1:B:312:ASP:CG	2.40	0.47
1:B:562:THR:OG1	1:B:661:LEU:HD22	2.15	0.47
1:C:102:GLY:CA	1:C:103:HIS:C	2.77	0.47
1:C:136:ARG:HD2	1:C:149:PHE:CE2	2.49	0.47
1:C:233:ASP:C	1:C:235:SER:H	2.23	0.47
1:C:308:HIS:HB3	1:C:312:ASP:CG	2.40	0.47
1:D:639:ILE:CG2	1:D:656:LEU:HD13	2.44	0.47
1:D:657:LEU:O	1:D:659:GLY:HA2	2.14	0.47
1:D:690:VAL:HA	1:D:693:VAL:HG13	1.97	0.47
1:A:131:TRP:N	1:A:132:PRO:CD	2.78	0.46
1:A:407:LEU:N	1:A:407:LEU:HD23	2.29	0.46
1:A:540:ALA:HB2	1:A:545:THR:HA	1.97	0.46
1:A:639:ILE:CG2	1:A:656:LEU:HD13	2.44	0.46
1:B:186:VAL:HG22	1:B:188:PHE:H	1.80	0.46
1:B:261:ASP:HB3	1:B:307:LEU:HB3	1.97	0.46
1:C:109:ILE:HG23	1:C:110:SER:CB	2.29	0.46
1:C:544:LYS:O	1:C:546:VAL:HG13	2.15	0.46
1:D:119:LEU:HD12	1:D:167:VAL:CG1	2.45	0.46
1:A:216:ILE:HD11	1:A:322:VAL:HG21	1.97	0.46
1:A:657:LEU:O	1:A:659:GLY:HA2	2.14	0.46
1:B:605:LYS:CE	1:B:628:ASP:HB3	2.43	0.46
1:C:216:ILE:HG21	1:C:326:GLN:HE22	1.79	0.46
1:C:539:MET:CE	1:C:547:ALA:HB3	2.45	0.46
1:D:146:LEU:HD13	1:D:344:VAL:HG22	1.97	0.46
1:A:119:LEU:HD12	1:A:167:VAL:CG1	2.46	0.46
1:B:131:TRP:N	1:B:132:PRO:CD	2.78	0.46
1:B:390:THR:N	1:B:391:PRO:HD2	2.30	0.46
1:B:460:HIS:HA	1:B:471:VAL:HG11	1.97	0.46
1:C:159:ALA:CB	1:C:379:ILE:HD13	2.42	0.46
1:C:261:ASP:HB3	1:C:307:LEU:HB3	1.98	0.46
1:C:540:ALA:HB2	1:C:545:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:THR:OG1	1:C:661:LEU:HD22	2.16	0.46
1:C:671:SER:O	1:C:672:GLU:C	2.57	0.46
1:D:414:LEU:HD23	1:D:414:LEU:HA	1.73	0.46
1:D:500:ASP:C	1:D:502:HIS:H	2.23	0.46
1:A:88:ALA:CB	1:A:125:VAL:HG23	2.46	0.46
1:A:308:HIS:HB3	1:A:312:ASP:CG	2.40	0.46
1:A:500:ASP:C	1:A:502:HIS:H	2.23	0.46
1:B:136:ARG:HD2	1:B:149:PHE:CE2	2.50	0.46
1:C:390:THR:N	1:C:391:PRO:HD2	2.30	0.46
1:C:574:VAL:HG22	1:C:595:LYS:HB2	1.97	0.46
1:D:490:PRO:HB2	1:D:493:LYS:HB2	1.98	0.46
1:D:544:LYS:O	1:D:546:VAL:HG13	2.15	0.46
1:A:713:ALA:O	1:A:717:MET:HG3	2.16	0.46
1:B:500:ASP:C	1:B:502:HIS:H	2.23	0.46
1:B:621:MET:CE	1:B:628:ASP:HB2	2.46	0.46
1:C:88:ALA:CB	1:C:125:VAL:HG23	2.46	0.46
1:C:119:LEU:HD12	1:C:167:VAL:CG1	2.45	0.46
1:D:109:ILE:HG23	1:D:110:SER:CB	2.30	0.46
1:D:367:LEU:C	1:D:367:LEU:HD22	2.40	0.46
1:D:455:ALA:HB2	1:D:539:MET:SD	2.55	0.46
1:D:708:LEU:HD13	1:D:709:SER:N	2.30	0.46
1:A:574:VAL:HG22	1:A:595:LYS:HB2	1.98	0.46
1:C:186:VAL:HG22	1:C:188:PHE:H	1.81	0.46
1:C:460:HIS:HA	1:C:471:VAL:HG11	1.97	0.46
1:C:621:MET:CE	1:C:628:ASP:HB2	2.46	0.46
1:D:308:HIS:HB3	1:D:312:ASP:CG	2.40	0.46
1:A:109:ILE:HG23	1:A:110:SER:CB	2.30	0.46
1:A:186:VAL:HG22	1:A:188:PHE:H	1.80	0.46
1:A:490:PRO:HB2	1:A:493:LYS:HB2	1.98	0.46
1:A:708:LEU:HD13	1:A:709:SER:N	2.30	0.46
1:B:216:ILE:HG21	1:B:326:GLN:HE22	1.79	0.46
1:B:540:ALA:HB2	1:B:545:THR:HA	1.97	0.46
1:C:131:TRP:N	1:C:132:PRO:CD	2.78	0.46
1:C:140:SER:HG	1:C:150:THR:HG22	1.81	0.46
1:C:605:LYS:CE	1:C:628:ASP:HB3	2.44	0.46
1:C:713:ALA:O	1:C:717:MET:HG3	2.16	0.46
1:B:109:ILE:HG23	1:B:110:SER:CB	2.30	0.46
1:B:363:PRO:HB2	1:B:364:GLN:CD	2.41	0.46
1:B:381:ALA:O	1:B:383:PRO:HD3	2.15	0.46
1:B:446:PHE:CE2	1:B:451:ALA:HB2	2.51	0.46
1:B:671:SER:O	1:B:672:GLU:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:ASN:O	1:B:730:ARG:HB3	2.16	0.46
1:C:179:SER:CB	1:C:183:VAL:HG22	2.46	0.46
1:C:500:ASP:C	1:C:502:HIS:H	2.23	0.46
1:C:559:THR:N	1:C:560:PRO:HD2	2.31	0.46
1:D:178:ARG:HB2	1:D:184:VAL:HA	1.98	0.46
1:D:186:VAL:HG22	1:D:188:PHE:H	1.80	0.46
1:A:178:ARG:HB2	1:A:184:VAL:HA	1.98	0.46
1:A:688:TYR:CD2	1:A:719:LEU:HB3	2.51	0.46
1:B:490:PRO:HB2	1:B:493:LYS:HB2	1.98	0.46
1:B:574:VAL:HG22	1:B:595:LYS:HB2	1.98	0.46
1:C:363:PRO:HB2	1:C:364:GLN:CD	2.41	0.46
1:C:381:ALA:O	1:C:383:PRO:HD3	2.16	0.46
1:C:490:PRO:HB2	1:C:493:LYS:HB2	1.98	0.46
1:D:363:PRO:HB2	1:D:364:GLN:CD	2.41	0.46
1:D:601:MET:HB3	1:D:602:PRO:HD2	1.97	0.46
1:A:422:THR:HG23	1:A:619:VAL:HG23	1.98	0.46
1:A:621:MET:CE	1:A:628:ASP:HB2	2.46	0.46
1:B:92:THR:O	1:B:95:VAL:HB	2.16	0.46
1:B:119:LEU:HD12	1:B:167:VAL:CG1	2.46	0.46
1:B:447:VAL:HG13	1:C:510:ARG:NH1	2.31	0.46
1:B:670:LEU:O	1:B:673:SER:HB3	2.16	0.46
1:C:164:MET:CE	1:C:164:MET:HA	2.46	0.46
1:C:427:LYS:HG3	1:C:428:THR:N	2.31	0.46
1:C:626:VAL:HA	1:C:647:VAL:HG22	1.98	0.46
1:D:88:ALA:CB	1:D:125:VAL:HG23	2.46	0.46
1:D:148:MET:HE3	1:D:149:PHE:CE1	2.51	0.46
1:D:574:VAL:HG22	1:D:595:LYS:HB2	1.98	0.46
1:D:621:MET:CE	1:D:628:ASP:HB2	2.46	0.46
1:D:688:TYR:CD2	1:D:719:LEU:HB3	2.51	0.46
1:D:688:TYR:CE1	1:D:719:LEU:HD23	2.50	0.46
1:A:446:PHE:CE2	1:A:451:ALA:HB2	2.51	0.45
1:A:544:LYS:O	1:A:546:VAL:HG13	2.15	0.45
1:A:629:ALA:HA	1:A:632:LEU:HD23	1.98	0.45
1:B:135:LYS:HG2	1:B:139:GLN:NE2	2.31	0.45
1:B:713:ALA:O	1:B:717:MET:HG3	2.16	0.45
1:C:178:ARG:HB2	1:C:184:VAL:HA	1.98	0.45
1:C:414:LEU:HA	1:C:414:LEU:HD23	1.73	0.45
1:D:179:SER:CB	1:D:183:VAL:HG22	2.45	0.45
1:A:148:MET:HE3	1:A:149:PHE:CE1	2.51	0.45
1:A:261:ASP:HB3	1:A:307:LEU:HB3	1.97	0.45
1:A:367:LEU:C	1:A:367:LEU:HD22	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:MET:HB3	1:A:602:PRO:HD2	1.98	0.45
1:B:626:VAL:HA	1:B:647:VAL:HG22	1.98	0.45
1:B:690:VAL:HA	1:B:693:VAL:HG13	1.97	0.45
1:C:127:LEU:C	1:C:129:GLY:N	2.72	0.45
1:C:135:LYS:HG2	1:C:139:GLN:NE2	2.31	0.45
1:D:261:ASP:HB3	1:D:307:LEU:HB3	1.97	0.45
1:D:297:ASN:C	1:D:298:GLN:HG3	2.41	0.45
1:D:406:VAL:C	1:D:407:LEU:HD23	2.42	0.45
1:D:422:THR:HG23	1:D:619:VAL:HG23	1.98	0.45
1:D:446:PHE:CE2	1:D:451:ALA:HB2	2.51	0.45
1:A:297:ASN:C	1:A:298:GLN:HG3	2.41	0.45
1:A:363:PRO:HB2	1:A:364:GLN:CD	2.41	0.45
1:A:440:ARG:O	1:A:550:VAL:HG22	2.16	0.45
1:B:164:MET:HA	1:B:164:MET:CE	2.46	0.45
1:B:178:ARG:HB2	1:B:184:VAL:HA	1.98	0.45
1:B:427:LYS:HG3	1:B:428:THR:N	2.31	0.45
1:B:690:VAL:O	1:B:694:PRO:HD3	2.16	0.45
1:D:670:LEU:O	1:D:673:SER:HB3	2.16	0.45
1:A:479:LEU:HD13	1:A:480:SER:H	1.81	0.45
1:B:440:ARG:O	1:B:550:VAL:HG22	2.16	0.45
1:C:178:ARG:HD3	1:C:178:ARG:HA	1.73	0.45
1:C:218:ALA:O	1:C:221:LYS:HB2	2.17	0.45
1:C:446:PHE:CE2	1:C:451:ALA:HB2	2.51	0.45
1:C:600:ILE:HD12	1:C:600:ILE:O	2.16	0.45
1:C:629:ALA:HA	1:C:632:LEU:HD23	1.99	0.45
1:D:440:ARG:O	1:D:550:VAL:HG22	2.16	0.45
1:D:727:ASN:O	1:D:730:ARG:HB3	2.16	0.45
1:A:406:VAL:C	1:A:407:LEU:HD23	2.42	0.45
1:A:460:HIS:HA	1:A:471:VAL:HG11	1.97	0.45
1:A:548:LEU:HD12	1:A:548:LEU:HA	1.77	0.45
1:A:562:THR:OG1	1:A:661:LEU:HD22	2.16	0.45
1:B:218:ALA:O	1:B:221:LYS:HB2	2.17	0.45
1:B:292:ILE:O	1:B:295:THR:HG22	2.16	0.45
1:B:539:MET:CE	1:B:547:ALA:HB3	2.46	0.45
1:C:292:ILE:O	1:C:295:THR:HG22	2.16	0.45
1:C:407:LEU:N	1:C:407:LEU:HD23	2.29	0.45
1:D:460:HIS:HA	1:D:471:VAL:HG11	1.97	0.45
1:D:562:THR:OG1	1:D:661:LEU:HD22	2.16	0.45
1:A:179:SER:CB	1:A:183:VAL:HG22	2.46	0.45
1:A:427:LYS:HG3	1:A:428:THR:N	2.30	0.45
1:A:559:THR:N	1:A:560:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:C	1:B:129:GLY:N	2.73	0.45
1:B:559:THR:N	1:B:560:PRO:HD2	2.32	0.45
1:C:392:MET:O	1:C:396:VAL:HG12	2.16	0.45
1:C:656:LEU:HD22	1:C:661:LEU:HA	1.98	0.45
1:D:135:LYS:HG2	1:D:139:GLN:NE2	2.31	0.45
1:D:629:ALA:HA	1:D:632:LEU:HD23	1.99	0.45
1:A:626:VAL:HA	1:A:647:VAL:HG22	1.97	0.45
1:B:178:ARG:HD3	1:B:178:ARG:HA	1.73	0.45
1:B:455:ALA:HB2	1:B:539:MET:SD	2.57	0.45
1:B:479:LEU:HD13	1:B:480:SER:H	1.82	0.45
1:B:600:ILE:HD12	1:B:600:ILE:O	2.17	0.45
1:B:629:ALA:HA	1:B:632:LEU:HD23	1.99	0.45
1:B:706:LEU:HB3	1:B:707:LEU:H	1.42	0.45
1:C:690:VAL:O	1:C:694:PRO:HD3	2.17	0.45
1:C:706:LEU:HB3	1:C:707:LEU:H	1.42	0.45
1:A:600:ILE:HD12	1:A:600:ILE:O	2.16	0.45
1:A:690:VAL:O	1:A:694:PRO:HD3	2.17	0.45
1:B:148:MET:HE3	1:B:149:PHE:CE1	2.52	0.45
1:B:297:ASN:C	1:B:298:GLN:HG3	2.41	0.45
1:B:711:MET:HE2	1:B:711:MET:HB2	1.91	0.45
1:C:148:MET:HE3	1:C:149:PHE:CE1	2.52	0.45
1:C:297:ASN:C	1:C:298:GLN:HG3	2.41	0.45
1:C:498:GLN:HG2	1:C:502:HIS:O	2.17	0.45
1:C:670:LEU:O	1:C:673:SER:HB3	2.17	0.45
1:C:688:TYR:CD2	1:C:719:LEU:HB3	2.51	0.45
1:D:343:PHE:O	1:D:347:VAL:HG23	2.17	0.45
1:D:626:VAL:HA	1:D:647:VAL:HG22	1.98	0.45
1:A:135:LYS:HG2	1:A:139:GLN:NE2	2.31	0.45
1:A:670:LEU:O	1:A:673:SER:HB3	2.17	0.45
1:C:440:ARG:O	1:C:550:VAL:HG22	2.16	0.45
1:D:479:LEU:HD13	1:D:480:SER:H	1.82	0.45
1:A:343:PHE:O	1:A:347:VAL:HG23	2.17	0.45
1:B:656:LEU:HD22	1:B:661:LEU:HA	1.98	0.45
1:C:343:PHE:O	1:C:347:VAL:HG23	2.16	0.45
1:C:461:GLN:CD	1:C:461:GLN:H	2.25	0.45
1:C:479:LEU:HD13	1:C:480:SER:H	1.82	0.45
1:C:524:GLU:HA	1:C:527:ASP:OD2	2.17	0.45
1:C:690:VAL:HA	1:C:693:VAL:HG13	1.98	0.45
1:D:427:LYS:HG3	1:D:428:THR:N	2.31	0.45
1:D:548:LEU:HD12	1:D:548:LEU:HA	1.77	0.45
1:A:656:LEU:HD22	1:A:661:LEU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ALA:O	1:B:125:VAL:HG12	2.17	0.44
1:B:407:LEU:N	1:B:407:LEU:HD23	2.30	0.44
1:B:491:THR:C	1:B:493:LYS:H	2.25	0.44
1:B:688:TYR:CD2	1:B:719:LEU:HB3	2.51	0.44
1:C:727:ASN:O	1:C:730:ARG:HB3	2.17	0.44
1:D:261:ASP:HA	1:D:293:GLY:N	2.33	0.44
1:D:392:MET:O	1:D:396:VAL:HG12	2.17	0.44
1:D:559:THR:N	1:D:560:PRO:HD2	2.32	0.44
1:D:600:ILE:HD12	1:D:600:ILE:O	2.17	0.44
1:A:261:ASP:HA	1:A:293:GLY:N	2.33	0.44
1:B:461:GLN:CD	1:B:461:GLN:H	2.26	0.44
1:B:479:LEU:HD13	1:B:480:SER:N	2.33	0.44
1:B:601:MET:HB3	1:B:602:PRO:HD2	1.98	0.44
1:C:230:ILE:HG12	1:C:235:SER:O	2.17	0.44
1:C:601:MET:HB3	1:C:602:PRO:HD2	1.98	0.44
1:C:711:MET:HE2	1:C:711:MET:HB2	1.92	0.44
1:D:430:THR:HG21	1:D:623:GLY:CA	2.43	0.44
1:A:727:ASN:O	1:A:730:ARG:HB3	2.17	0.44
1:B:88:ALA:CB	1:B:125:VAL:HG23	2.47	0.44
1:B:230:ILE:HG12	1:B:235:SER:O	2.17	0.44
1:B:422:THR:HG23	1:B:619:VAL:HG23	1.98	0.44
1:B:498:GLN:HG2	1:B:502:HIS:O	2.17	0.44
1:C:317:ARG:HH21	1:C:603:GLU:CD	2.26	0.44
1:C:450:ASN:O	1:C:454:LEU:HG	2.17	0.44
1:C:491:THR:C	1:C:493:LYS:H	2.25	0.44
1:D:690:VAL:O	1:D:694:PRO:HD3	2.17	0.44
1:A:218:ALA:O	1:A:221:LYS:HB2	2.17	0.44
1:A:292:ILE:O	1:A:295:THR:HG22	2.17	0.44
1:A:450:ASN:O	1:A:454:LEU:HG	2.18	0.44
1:A:498:GLN:HG2	1:A:502:HIS:O	2.17	0.44
1:B:317:ARG:HH21	1:B:603:GLU:CD	2.26	0.44
1:B:392:MET:O	1:B:396:VAL:HG12	2.17	0.44
1:B:450:ASN:O	1:B:454:LEU:HG	2.17	0.44
1:C:406:VAL:C	1:C:407:LEU:HD23	2.42	0.44
1:D:218:ALA:O	1:D:221:LYS:HB2	2.17	0.44
1:D:381:ALA:O	1:D:383:PRO:HD3	2.16	0.44
1:D:413:ALA:HB1	1:D:654:VAL:HG23	1.99	0.44
1:D:461:GLN:H	1:D:461:GLN:CD	2.25	0.44
1:D:468:ASN:O	1:D:472:HIS:HB2	2.18	0.44
1:D:498:GLN:HG2	1:D:502:HIS:O	2.17	0.44
1:D:656:LEU:HD22	1:D:661:LEU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:O	1:A:125:VAL:HG12	2.17	0.44
1:A:392:MET:O	1:A:396:VAL:HG12	2.17	0.44
1:A:468:ASN:O	1:A:472:HIS:HB2	2.18	0.44
1:B:343:PHE:O	1:B:347:VAL:HG23	2.17	0.44
1:D:450:ASN:O	1:D:454:LEU:HG	2.18	0.44
1:A:430:THR:HG21	1:A:623:GLY:CA	2.44	0.44
1:A:461:GLN:H	1:A:461:GLN:CD	2.26	0.44
1:B:219:LEU:HD22	1:B:647:VAL:HG12	2.00	0.44
1:C:122:ALA:O	1:C:125:VAL:HG12	2.18	0.44
1:C:479:LEU:HD13	1:C:480:SER:N	2.33	0.44
1:D:292:ILE:O	1:D:295:THR:HG22	2.17	0.44
1:D:500:ASP:C	1:D:502:HIS:N	2.76	0.44
1:A:156:ILE:HD11	1:A:194:ILE:CG2	2.48	0.44
1:A:230:ILE:HG12	1:A:235:SER:O	2.17	0.44
1:A:381:ALA:O	1:A:383:PRO:HD3	2.17	0.44
1:A:500:ASP:C	1:A:502:HIS:N	2.76	0.44
1:A:699:VAL:HG23	1:A:700:LEU:HD23	1.99	0.44
1:B:168:LEU:HD12	1:B:168:LEU:HA	1.86	0.44
1:B:277:THR:CG2	1:B:578:GLY:O	2.66	0.44
1:B:413:ALA:HB1	1:B:654:VAL:HG23	1.99	0.44
1:B:430:THR:HG21	1:B:623:GLY:CA	2.43	0.44
1:B:524:GLU:HA	1:B:527:ASP:OD2	2.18	0.44
1:D:156:ILE:HD11	1:D:194:ILE:CG2	2.48	0.44
1:D:164:MET:HA	1:D:164:MET:CE	2.48	0.44
1:A:179:SER:N	1:A:180:GLN:CA	2.81	0.44
1:A:277:THR:CG2	1:A:578:GLY:O	2.66	0.44
1:A:313:THR:HG22	1:A:316:ALA:HB3	1.98	0.44
1:B:78:TYR:CD2	1:B:79:LEU:HD12	2.42	0.44
1:B:261:ASP:HA	1:B:293:GLY:N	2.33	0.44
1:B:406:VAL:C	1:B:407:LEU:HD23	2.43	0.44
1:B:490:PRO:HD2	1:B:495:VAL:HA	1.99	0.44
1:C:178:ARG:CB	1:C:179:SER:HA	2.24	0.44
1:C:219:LEU:HD22	1:C:647:VAL:HG12	2.00	0.44
1:C:261:ASP:HA	1:C:293:GLY:N	2.33	0.44
1:C:313:THR:HG22	1:C:316:ALA:HB3	1.98	0.44
1:D:179:SER:N	1:D:180:GLN:CA	2.81	0.44
1:D:221:LYS:O	1:D:222:LEU:C	2.61	0.44
1:D:230:ILE:HG12	1:D:235:SER:O	2.17	0.44
1:D:498:GLN:HA	1:D:502:HIS:O	2.18	0.44
1:A:221:LYS:O	1:A:222:LEU:C	2.61	0.44
1:A:491:THR:C	1:A:493:LYS:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:HIS:HA	1:B:104:GLY:HA3	1.78	0.44
1:B:140:SER:HG	1:B:150:THR:HG22	1.83	0.44
1:B:178:ARG:CB	1:B:179:SER:HA	2.24	0.44
1:B:313:THR:HG22	1:B:316:ALA:HB3	1.98	0.44
1:B:498:GLN:HA	1:B:502:HIS:O	2.18	0.44
1:B:627:ASN:C	1:B:629:ALA:H	2.26	0.44
1:B:703:LEU:CD2	1:D:86:TRP:HB2	2.48	0.44
1:C:78:TYR:CD2	1:C:79:LEU:HD12	2.42	0.44
1:C:413:ALA:HB1	1:C:654:VAL:HG23	1.99	0.44
1:D:326:GLN:O	1:D:329:ARG:HG3	2.18	0.44
1:A:228:HIS:O	1:A:250:LEU:HD22	2.18	0.43
1:A:326:GLN:O	1:A:329:ARG:HG3	2.18	0.43
1:A:455:ALA:HB2	1:A:539:MET:SD	2.58	0.43
1:C:103:HIS:HA	1:C:104:GLY:HA3	1.78	0.43
1:C:422:THR:HG23	1:C:619:VAL:HG23	1.99	0.43
1:C:455:ALA:HB2	1:C:539:MET:SD	2.58	0.43
1:C:627:ASN:C	1:C:629:ALA:H	2.27	0.43
1:D:122:ALA:O	1:D:125:VAL:HG12	2.18	0.43
1:D:277:THR:CG2	1:D:578:GLY:O	2.66	0.43
1:D:491:THR:C	1:D:493:LYS:H	2.25	0.43
1:D:699:VAL:HG23	1:D:700:LEU:HD23	2.00	0.43
1:A:313:THR:HG23	1:A:316:ALA:H	1.83	0.43
1:B:122:ALA:HA	1:B:125:VAL:CG1	2.47	0.43
1:B:414:LEU:HD23	1:B:414:LEU:HA	1.73	0.43
1:B:416:ARG:HG2	1:B:416:ARG:HH11	1.82	0.43
1:B:468:ASN:O	1:B:472:HIS:HB2	2.18	0.43
1:C:168:LEU:HD12	1:C:168:LEU:HA	1.86	0.43
1:C:430:THR:HG21	1:C:623:GLY:CA	2.43	0.43
1:C:490:PRO:HD2	1:C:495:VAL:HA	2.00	0.43
1:D:228:HIS:O	1:D:250:LEU:HD22	2.18	0.43
1:D:313:THR:HG22	1:D:316:ALA:HB3	1.98	0.43
1:D:313:THR:HG23	1:D:316:ALA:H	1.83	0.43
1:D:500:ASP:OD1	1:D:500:ASP:C	2.61	0.43
1:D:660:ASP:C	1:D:662:ARG:N	2.75	0.43
1:A:498:GLN:HA	1:A:502:HIS:O	2.18	0.43
1:A:500:ASP:OD1	1:A:500:ASP:C	2.61	0.43
1:A:524:GLU:HA	1:A:527:ASP:OD2	2.17	0.43
1:B:221:LYS:O	1:B:222:LEU:C	2.60	0.43
1:C:122:ALA:HA	1:C:125:VAL:CG1	2.47	0.43
1:C:221:LYS:O	1:C:222:LEU:C	2.60	0.43
1:D:206:LEU:O	1:D:210:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:VAL:O	1:D:277:THR:CB	2.67	0.43
1:D:317:ARG:HH21	1:D:603:GLU:CD	2.26	0.43
1:A:164:MET:CE	1:A:164:MET:HA	2.48	0.43
1:A:317:ARG:HH21	1:A:603:GLU:CD	2.26	0.43
1:A:413:ALA:HB1	1:A:654:VAL:HG23	2.00	0.43
1:A:416:ARG:HG2	1:A:416:ARG:HH11	1.82	0.43
1:A:479:LEU:HD13	1:A:480:SER:N	2.33	0.43
1:B:307:LEU:HD13	1:B:308:HIS:CD2	2.49	0.43
1:C:307:LEU:HD13	1:C:308:HIS:CD2	2.49	0.43
1:D:490:PRO:HD2	1:D:495:VAL:HA	1.99	0.43
1:A:206:LEU:O	1:A:210:GLU:HB2	2.19	0.43
1:A:490:PRO:HD2	1:A:495:VAL:HA	2.00	0.43
1:A:660:ASP:C	1:A:662:ARG:N	2.75	0.43
1:B:447:VAL:HG23	1:B:450:ASN:H	1.83	0.43
1:B:500:ASP:C	1:B:502:HIS:N	2.76	0.43
1:C:86:TRP:O	1:C:90:MET:HG3	2.18	0.43
1:C:468:ASN:O	1:C:472:HIS:HB2	2.18	0.43
1:C:699:VAL:HG23	1:C:700:LEU:HD23	1.99	0.43
1:D:416:ARG:HG2	1:D:416:ARG:HH11	1.82	0.43
1:A:127:LEU:C	1:A:129:GLY:N	2.73	0.43
1:A:183:VAL:HG23	1:A:184:VAL:N	2.33	0.43
1:A:276:VAL:O	1:A:277:THR:CB	2.67	0.43
1:C:156:ILE:HD11	1:C:194:ILE:CG2	2.48	0.43
1:C:326:GLN:O	1:C:329:ARG:HG3	2.18	0.43
1:D:86:TRP:O	1:D:90:MET:HG3	2.18	0.43
1:D:179:SER:HB3	1:D:182:GLY:N	2.34	0.43
1:A:447:VAL:HG23	1:A:450:ASN:H	1.84	0.43
1:B:156:ILE:HD11	1:B:194:ILE:CG2	2.48	0.43
1:B:326:GLN:O	1:B:329:ARG:HG3	2.18	0.43
1:B:500:ASP:OD1	1:B:500:ASP:C	2.61	0.43
1:B:660:ASP:C	1:B:662:ARG:N	2.75	0.43
1:C:166:ALA:HB1	1:C:184:VAL:CG2	2.49	0.43
1:C:168:LEU:HD23	1:C:169:TRP:CZ3	2.54	0.43
1:C:447:VAL:HG23	1:C:450:ASN:H	1.84	0.43
1:C:576:LEU:HB3	1:C:605:LYS:HZ2	1.84	0.43
1:D:447:VAL:HG23	1:D:450:ASN:H	1.84	0.43
1:D:479:LEU:HD13	1:D:480:SER:N	2.33	0.43
1:D:524:GLU:HA	1:D:527:ASP:OD2	2.17	0.43
1:D:617:LEU:O	1:D:618:ILE:C	2.62	0.43
1:A:86:TRP:O	1:A:90:MET:HG3	2.18	0.43
1:A:627:ASN:C	1:A:629:ALA:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:ARG:CZ	1:A:736:LEU:O	2.67	0.43
1:B:249:LEU:HA	1:B:304:MET:O	2.19	0.43
1:B:699:VAL:HG23	1:B:700:LEU:HD23	2.00	0.43
1:C:179:SER:N	1:C:180:GLN:CA	2.80	0.43
1:C:500:ASP:OD1	1:C:500:ASP:C	2.61	0.43
1:C:500:ASP:C	1:C:502:HIS:N	2.76	0.43
1:D:249:LEU:HA	1:D:304:MET:O	2.19	0.43
1:D:277:THR:HG23	1:D:578:GLY:O	2.19	0.43
1:D:669:ARG:CZ	1:D:736:LEU:O	2.67	0.43
1:A:277:THR:HG23	1:A:578:GLY:O	2.19	0.43
1:A:617:LEU:O	1:A:618:ILE:C	2.62	0.43
1:B:168:LEU:HD23	1:B:169:TRP:CZ3	2.54	0.43
1:B:576:LEU:HB3	1:B:605:LYS:HZ2	1.84	0.43
1:C:249:LEU:HA	1:C:304:MET:O	2.19	0.43
1:D:627:ASN:C	1:D:629:ALA:H	2.26	0.43
1:A:122:ALA:HA	1:A:125:VAL:CG1	2.46	0.43
1:A:168:LEU:HD23	1:A:169:TRP:CZ3	2.54	0.43
1:A:249:LEU:HA	1:A:304:MET:O	2.19	0.43
1:C:277:THR:CG2	1:C:578:GLY:O	2.67	0.43
1:C:416:ARG:HH11	1:C:416:ARG:HG2	1.83	0.43
1:C:498:GLN:HA	1:C:502:HIS:O	2.19	0.43
1:A:262:GLY:CA	1:A:305:LYS:O	2.67	0.42
1:B:86:TRP:O	1:B:90:MET:HG3	2.19	0.42
1:B:179:SER:N	1:B:180:GLN:CA	2.81	0.42
1:B:228:HIS:O	1:B:250:LEU:HD22	2.18	0.42
1:B:262:GLY:CA	1:B:307:LEU:HB2	2.49	0.42
1:B:277:THR:HG23	1:B:578:GLY:O	2.19	0.42
1:B:559:THR:O	1:B:563:ILE:HG12	2.19	0.42
1:C:228:HIS:O	1:C:250:LEU:HD22	2.18	0.42
1:D:122:ALA:HA	1:D:125:VAL:CG1	2.46	0.42
1:D:127:LEU:C	1:D:129:GLY:N	2.73	0.42
1:D:168:LEU:HD23	1:D:169:TRP:CZ3	2.54	0.42
1:D:183:VAL:HG23	1:D:184:VAL:N	2.34	0.42
1:B:148:MET:SD	1:B:386:LEU:HD13	2.59	0.42
1:C:179:SER:HB3	1:C:182:GLY:N	2.34	0.42
1:C:559:THR:O	1:C:563:ILE:HG12	2.19	0.42
1:D:219:LEU:HD22	1:D:647:VAL:HG12	2.00	0.42
1:D:262:GLY:CA	1:D:305:LYS:O	2.67	0.42
1:D:559:THR:O	1:D:563:ILE:HG12	2.19	0.42
1:A:179:SER:HB3	1:A:182:GLY:N	2.35	0.42
1:B:539:MET:HE2	1:B:539:MET:HB3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:MET:SD	1:C:386:LEU:HD13	2.59	0.42
1:C:183:VAL:HG23	1:C:184:VAL:N	2.33	0.42
1:C:244:VAL:HG12	1:C:245:ALA:N	2.35	0.42
1:C:313:THR:HG23	1:C:316:ALA:H	1.83	0.42
1:C:600:ILE:HB	1:C:604:ASP:CG	2.45	0.42
1:C:731:LEU:O	1:C:731:LEU:HD13	2.20	0.42
1:D:148:MET:SD	1:D:386:LEU:HD13	2.59	0.42
1:D:272:ASP:HB3	1:D:296:ILE:HG23	2.01	0.42
1:A:219:LEU:HD22	1:A:647:VAL:HG12	2.00	0.42
1:B:179:SER:HB3	1:B:182:GLY:N	2.35	0.42
1:B:244:VAL:HG12	1:B:245:ALA:N	2.35	0.42
1:B:313:THR:HG23	1:B:316:ALA:H	1.83	0.42
1:B:600:ILE:HB	1:B:604:ASP:CG	2.45	0.42
1:C:122:ALA:CA	1:C:125:VAL:HG12	2.47	0.42
1:C:660:ASP:C	1:C:662:ARG:N	2.76	0.42
1:C:730:ARG:HG3	1:C:730:ARG:HH11	1.84	0.42
1:A:168:LEU:HA	1:A:168:LEU:HD12	1.86	0.42
1:A:244:VAL:HG12	1:A:245:ALA:N	2.35	0.42
1:B:166:ALA:HB1	1:B:184:VAL:CG2	2.50	0.42
1:B:264:VAL:HG22	1:B:287:ALA:HA	2.01	0.42
1:C:264:VAL:HG22	1:C:287:ALA:HA	2.01	0.42
1:D:262:GLY:CA	1:D:307:LEU:HB2	2.49	0.42
1:A:332:ILE:HD12	1:A:332:ILE:HA	1.93	0.42
1:B:122:ALA:CA	1:B:125:VAL:HG12	2.48	0.42
1:B:708:LEU:HD13	1:B:708:LEU:C	2.45	0.42
1:C:276:VAL:O	1:C:277:THR:CB	2.66	0.42
1:C:539:MET:HE2	1:C:539:MET:HB3	1.86	0.42
1:D:244:VAL:HG12	1:D:245:ALA:N	2.35	0.42
1:D:277:THR:HG22	1:D:279:GLU:HG2	2.02	0.42
1:D:600:ILE:HB	1:D:604:ASP:CG	2.45	0.42
1:A:262:GLY:CA	1:A:307:LEU:HB2	2.50	0.42
1:A:600:ILE:HB	1:A:604:ASP:CG	2.45	0.42
1:B:179:SER:HB3	1:B:180:GLN:C	2.45	0.42
1:B:206:LEU:O	1:B:210:GLU:HB2	2.19	0.42
1:B:271:VAL:HA	1:B:297:ASN:HA	2.02	0.42
1:B:418:GLU:CG	1:B:672:GLU:HG2	2.47	0.42
1:B:605:LYS:HD3	1:B:628:ASP:CB	2.50	0.42
1:B:669:ARG:CZ	1:B:736:LEU:O	2.67	0.42
1:B:730:ARG:HH11	1:B:730:ARG:HG3	1.85	0.42
1:C:418:GLU:CG	1:C:672:GLU:HG2	2.47	0.42
1:C:454:LEU:HD22	1:C:499:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LEU:HA	1:D:188:PHE:CE2	2.55	0.42
1:D:418:GLU:CG	1:D:672:GLU:HG2	2.47	0.42
1:D:428:THR:O	2:D:995:ALF:F2	2.28	0.42
1:D:642:GLY:O	1:D:645:THR:HG22	2.20	0.42
1:A:272:ASP:HB3	1:A:296:ILE:HG23	2.02	0.42
1:A:559:THR:O	1:A:563:ILE:HG12	2.19	0.42
1:B:467:ALA:O	1:B:471:VAL:HG13	2.20	0.42
1:C:88:ALA:HB1	1:C:125:VAL:HG23	2.02	0.42
1:C:91:LEU:O	1:C:95:VAL:HG23	2.20	0.42
1:C:669:ARG:CZ	1:C:736:LEU:O	2.67	0.42
1:C:708:LEU:HD13	1:C:708:LEU:C	2.45	0.42
1:C:734:VAL:HG22	1:C:734:VAL:O	2.20	0.42
1:D:332:ILE:HD12	1:D:332:ILE:HA	1.93	0.42
1:A:148:MET:SD	1:A:386:LEU:HD13	2.60	0.42
1:A:539:MET:HE2	1:A:539:MET:HB3	1.87	0.42
1:A:642:GLY:O	1:A:645:THR:HG22	2.20	0.42
1:A:734:VAL:O	1:A:734:VAL:HG22	2.20	0.42
1:B:454:LEU:HD22	1:B:499:VAL:CG1	2.50	0.42
1:B:617:LEU:O	1:B:618:ILE:C	2.61	0.42
1:B:731:LEU:HD13	1:B:731:LEU:O	2.20	0.42
1:C:127:LEU:O	1:C:131:TRP:HB2	2.19	0.42
1:C:179:SER:HB3	1:C:180:GLN:C	2.45	0.42
1:C:271:VAL:HA	1:C:297:ASN:HA	2.02	0.42
1:C:642:GLY:O	1:C:645:THR:HG22	2.20	0.42
1:D:676:SER:O	1:D:680:GLN:HG3	2.20	0.42
1:A:86:TRP:HB2	1:C:703:LEU:CD2	2.50	0.42
1:A:271:VAL:HA	1:A:297:ASN:HA	2.02	0.42
1:A:422:THR:O	1:A:619:VAL:HG23	2.20	0.42
1:A:443:THR:HG21	1:A:446:PHE:O	2.20	0.42
1:A:730:ARG:HG3	1:A:730:ARG:HH11	1.85	0.42
1:B:173:PHE:HA	1:B:174:PRO:HD3	1.87	0.42
1:B:183:VAL:HG23	1:B:184:VAL:N	2.34	0.42
1:B:224:PRO:HG3	1:B:257:LYS:HD2	2.01	0.42
1:B:355:PHE:O	1:B:359:ALA:HB2	2.20	0.42
1:B:499:VAL:O	1:B:502:HIS:ND1	2.53	0.42
1:C:224:PRO:HG3	1:C:257:LYS:HD2	2.01	0.42
1:D:499:VAL:O	1:D:502:HIS:ND1	2.53	0.42
1:A:84:ARG:NH1	1:A:132:PRO:HD3	2.35	0.41
1:A:119:LEU:HA	1:A:188:PHE:CE2	2.55	0.41
1:A:127:LEU:O	1:A:131:TRP:HB2	2.19	0.41
1:A:264:VAL:HG22	1:A:287:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:PHE:O	1:A:359:ALA:HB2	2.20	0.41
1:B:642:GLY:O	1:B:645:THR:HG22	2.20	0.41
1:C:173:PHE:HA	1:C:174:PRO:HD3	1.87	0.41
1:D:264:VAL:HG22	1:D:287:ALA:HA	2.01	0.41
1:D:271:VAL:HA	1:D:297:ASN:HA	2.02	0.41
1:D:731:LEU:HD13	1:D:731:LEU:O	2.20	0.41
1:A:129:GLY:HA3	1:A:130:GLY:HA3	1.70	0.41
1:A:151:LEU:HD13	1:A:344:VAL:HG12	2.02	0.41
1:C:442:VAL:HG23	1:C:548:LEU:HB3	2.02	0.41
1:C:605:LYS:HD3	1:C:628:ASP:CB	2.51	0.41
1:D:84:ARG:NH1	1:D:132:PRO:HD3	2.36	0.41
1:D:355:PHE:O	1:D:359:ALA:HB2	2.20	0.41
1:A:166:ALA:HB1	1:A:184:VAL:CG2	2.50	0.41
1:A:224:PRO:HG3	1:A:257:LYS:HD2	2.01	0.41
1:A:454:LEU:HD22	1:A:499:VAL:CG1	2.50	0.41
1:A:467:ALA:O	1:A:471:VAL:HG13	2.21	0.41
1:B:127:LEU:O	1:B:131:TRP:HB2	2.20	0.41
1:B:262:GLY:CA	1:B:305:LYS:O	2.67	0.41
1:B:695:LEU:O	1:B:707:LEU:HG	2.20	0.41
1:B:734:VAL:HG22	1:B:734:VAL:O	2.20	0.41
1:C:355:PHE:O	1:C:359:ALA:HB2	2.21	0.41
1:C:499:VAL:O	1:C:502:HIS:ND1	2.53	0.41
1:D:151:LEU:HD13	1:D:344:VAL:HG12	2.02	0.41
1:D:224:PRO:HG3	1:D:257:LYS:HD2	2.01	0.41
1:D:734:VAL:O	1:D:734:VAL:HG22	2.20	0.41
1:A:253:ARG:HD2	1:A:254:PRO:O	2.21	0.41
1:A:499:VAL:O	1:A:502:HIS:CA	2.69	0.41
1:B:276:VAL:O	1:B:277:THR:CB	2.67	0.41
1:C:262:GLY:CA	1:C:305:LYS:O	2.67	0.41
1:C:277:THR:HG23	1:C:578:GLY:O	2.20	0.41
1:C:558:SER:C	1:C:560:PRO:HD2	2.46	0.41
1:D:168:LEU:HD12	1:D:168:LEU:HA	1.87	0.41
1:D:499:VAL:O	1:D:502:HIS:CA	2.69	0.41
1:A:277:THR:HG22	1:A:279:GLU:HG2	2.03	0.41
1:A:408:ILE:HD12	1:A:408:ILE:N	2.35	0.41
1:A:731:LEU:HD13	1:A:731:LEU:O	2.20	0.41
1:B:272:ASP:HB3	1:B:296:ILE:HG23	2.01	0.41
1:B:442:VAL:HG23	1:B:548:LEU:HB3	2.03	0.41
1:B:499:VAL:O	1:B:502:HIS:CA	2.69	0.41
1:C:408:ILE:HD12	1:C:408:ILE:N	2.36	0.41
1:D:605:LYS:HD3	1:D:628:ASP:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD12	1:A:249:LEU:N	2.36	0.41
1:A:499:VAL:O	1:A:502:HIS:ND1	2.53	0.41
1:B:253:ARG:HD2	1:B:254:PRO:O	2.20	0.41
1:C:467:ALA:O	1:C:471:VAL:HG13	2.21	0.41
1:D:127:LEU:O	1:D:131:TRP:HB2	2.20	0.41
1:D:249:LEU:N	1:D:249:LEU:HD12	2.36	0.41
1:D:443:THR:HG21	1:D:446:PHE:O	2.20	0.41
1:D:467:ALA:O	1:D:471:VAL:HG13	2.21	0.41
1:D:629:ALA:N	1:D:630:PRO:CD	2.82	0.41
1:D:695:LEU:O	1:D:707:LEU:HG	2.21	0.41
1:D:730:ARG:HG3	1:D:730:ARG:HH11	1.86	0.41
1:A:277:THR:HG23	1:A:578:GLY:C	2.46	0.41
1:A:605:LYS:HD3	1:A:628:ASP:CB	2.51	0.41
1:A:629:ALA:N	1:A:630:PRO:CD	2.82	0.41
1:B:84:ARG:NH1	1:B:132:PRO:HD3	2.35	0.41
1:C:206:LEU:O	1:C:210:GLU:HB2	2.20	0.41
1:C:277:THR:HG22	1:C:279:GLU:HG2	2.03	0.41
1:C:490:PRO:CB	1:C:493:LYS:HD3	2.49	0.41
1:C:499:VAL:O	1:C:502:HIS:CA	2.69	0.41
1:C:617:LEU:O	1:C:618:ILE:C	2.63	0.41
1:D:253:ARG:HD2	1:D:254:PRO:O	2.21	0.41
1:D:576:LEU:C	1:D:605:LYS:HZ1	2.29	0.41
1:A:692:GLY:C	1:A:694:PRO:HD2	2.46	0.41
1:B:119:LEU:HA	1:B:188:PHE:CE2	2.55	0.41
1:B:219:LEU:HD21	1:B:647:VAL:HA	2.02	0.41
1:B:312:ASP:OD2	1:B:312:ASP:N	2.53	0.41
1:B:431:LEU:HD12	1:B:431:LEU:HA	1.93	0.41
1:B:490:PRO:CB	1:B:493:LYS:HD3	2.49	0.41
1:C:253:ARG:HD2	1:C:254:PRO:O	2.21	0.41
1:C:422:THR:O	1:C:619:VAL:HG23	2.21	0.41
1:D:93:ILE:HG23	1:D:94:PRO:CD	2.48	0.41
1:D:454:LEU:HD22	1:D:499:VAL:CG1	2.51	0.41
1:A:93:ILE:HG23	1:A:94:PRO:CD	2.49	0.41
1:A:154:MET:HE2	1:A:154:MET:HB3	1.99	0.41
1:A:173:PHE:HA	1:A:174:PRO:HD3	1.87	0.41
1:A:307:LEU:HD13	1:A:308:HIS:CD2	2.48	0.41
1:A:695:LEU:O	1:A:707:LEU:HG	2.21	0.41
1:B:233:ASP:C	1:B:235:SER:N	2.79	0.41
1:B:408:ILE:N	1:B:408:ILE:HD12	2.36	0.41
1:B:426:ASP:HA	1:B:576:LEU:O	2.21	0.41
1:B:438:LEU:HD12	1:B:473:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:ASP:C	1:B:662:ARG:H	2.29	0.41
1:C:84:ARG:NH1	1:C:132:PRO:HD3	2.36	0.41
1:C:219:LEU:HD21	1:C:647:VAL:HA	2.02	0.41
1:C:233:ASP:C	1:C:235:SER:N	2.79	0.41
1:C:312:ASP:OD2	1:C:312:ASP:N	2.53	0.41
1:C:431:LEU:HD12	1:C:431:LEU:HA	1.93	0.41
1:C:628:ASP:O	1:C:631:ALA:HB3	2.20	0.41
1:C:660:ASP:C	1:C:662:ARG:H	2.29	0.41
1:C:695:LEU:O	1:C:707:LEU:HG	2.21	0.41
1:D:129:GLY:HA3	1:D:130:GLY:HA3	1.70	0.41
1:D:166:ALA:HB1	1:D:184:VAL:CG2	2.51	0.41
1:D:173:PHE:HA	1:D:174:PRO:HD3	1.87	0.41
1:D:277:THR:HG23	1:D:578:GLY:C	2.46	0.41
1:D:307:LEU:HD13	1:D:308:HIS:CD2	2.49	0.41
1:D:539:MET:HE2	1:D:539:MET:HB3	1.87	0.41
1:D:574:VAL:O	1:D:574:VAL:HG12	2.21	0.41
1:D:708:LEU:HD13	1:D:708:LEU:C	2.45	0.41
1:A:117:ILE:HG12	1:C:687:ILE:HD11	2.03	0.41
1:A:155:GLY:O	1:A:159:ALA:HB2	2.21	0.41
1:A:708:LEU:HD13	1:A:708:LEU:C	2.45	0.41
1:B:277:THR:HG22	1:B:279:GLU:HG2	2.03	0.41
1:B:574:VAL:O	1:B:574:VAL:HG12	2.21	0.41
1:B:692:GLY:C	1:B:694:PRO:HD2	2.45	0.41
1:C:119:LEU:HA	1:C:188:PHE:CE2	2.56	0.41
1:C:272:ASP:HB3	1:C:296:ILE:HG23	2.02	0.41
1:A:85:PHE:CE1	1:A:200:LEU:HB2	2.56	0.40
1:A:251:ARG:HA	1:A:302:PHE:O	2.21	0.40
1:A:442:VAL:HG23	1:A:548:LEU:HB3	2.03	0.40
1:A:576:LEU:C	1:A:605:LYS:HZ1	2.30	0.40
1:A:676:SER:O	1:A:680:GLN:HG3	2.21	0.40
1:B:223:VAL:HG12	1:B:225:GLU:HB3	2.03	0.40
1:B:249:LEU:HD12	1:B:249:LEU:N	2.36	0.40
1:B:251:ARG:HA	1:B:302:PHE:O	2.21	0.40
1:B:277:THR:HG23	1:B:578:GLY:C	2.46	0.40
1:B:558:SER:C	1:B:560:PRO:HD2	2.47	0.40
1:C:223:VAL:HG12	1:C:225:GLU:HB3	2.03	0.40
1:C:249:LEU:HD12	1:C:249:LEU:N	2.36	0.40
1:C:426:ASP:OD2	2:C:995:ALF:F2	2.29	0.40
1:C:443:THR:HG21	1:C:446:PHE:O	2.20	0.40
1:C:576:LEU:HB3	1:C:605:LYS:NZ	2.36	0.40
1:C:692:GLY:C	1:C:694:PRO:HD2	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:PHE:CE1	1:D:200:LEU:HB2	2.56	0.40
1:D:219:LEU:HD21	1:D:647:VAL:HA	2.02	0.40
1:D:408:ILE:HD12	1:D:408:ILE:N	2.36	0.40
1:A:276:VAL:C	1:A:278:GLY:H	2.29	0.40
1:B:131:TRP:N	1:B:132:PRO:HD2	2.36	0.40
1:B:155:GLY:O	1:B:159:ALA:HB2	2.21	0.40
1:B:422:THR:O	1:B:619:VAL:HG23	2.22	0.40
1:B:576:LEU:HB3	1:B:605:LYS:NZ	2.36	0.40
1:C:251:ARG:HA	1:C:302:PHE:O	2.21	0.40
1:C:438:LEU:HD12	1:C:473:ALA:CB	2.51	0.40
1:C:522:LEU:HD12	1:C:545:THR:HG22	2.03	0.40
1:D:131:TRP:N	1:D:132:PRO:HD2	2.35	0.40
1:D:276:VAL:C	1:D:278:GLY:H	2.29	0.40
1:D:522:LEU:HD12	1:D:545:THR:HG22	2.03	0.40
1:D:692:GLY:C	1:D:694:PRO:HD2	2.46	0.40
1:A:233:ASP:C	1:A:235:SER:N	2.79	0.40
1:A:522:LEU:HD12	1:A:545:THR:HG22	2.03	0.40
1:B:85:PHE:CE1	1:B:200:LEU:HB2	2.57	0.40
1:B:276:VAL:C	1:B:278:GLY:H	2.29	0.40
1:C:131:TRP:N	1:C:132:PRO:HD2	2.36	0.40
1:C:426:ASP:HA	1:C:576:LEU:O	2.21	0.40
1:D:154:MET:HE2	1:D:154:MET:HB3	2.00	0.40
1:D:179:SER:HB3	1:D:180:GLN:C	2.45	0.40
1:D:233:ASP:C	1:D:235:SER:N	2.79	0.40
1:D:251:ARG:HA	1:D:302:PHE:O	2.22	0.40
1:D:422:THR:O	1:D:619:VAL:HG23	2.22	0.40
1:A:91:LEU:O	1:A:95:VAL:HG23	2.21	0.40
1:A:219:LEU:HD21	1:A:647:VAL:HA	2.03	0.40
1:A:394:ILE:O	1:A:398:VAL:HG13	2.22	0.40
1:B:522:LEU:HD12	1:B:545:THR:HG22	2.04	0.40
1:C:574:VAL:O	1:C:574:VAL:HG12	2.21	0.40
1:D:438:LEU:HD12	1:D:473:ALA:CB	2.51	0.40
1:A:88:ALA:HB1	1:A:125:VAL:HG23	2.02	0.40
1:A:131:TRP:N	1:A:132:PRO:HD2	2.36	0.40
1:A:179:SER:HB3	1:A:180:GLN:C	2.45	0.40
1:A:258:ILE:HD11	1:A:297:ASN:HB3	2.03	0.40
1:A:438:LEU:HD12	1:A:473:ALA:CB	2.51	0.40
1:B:88:ALA:HB1	1:B:125:VAL:HG23	2.04	0.40
1:B:258:ILE:HA	1:B:259:PRO:HD3	1.82	0.40
1:C:276:VAL:C	1:C:278:GLY:H	2.29	0.40
1:D:130:GLY:HA2	1:D:133:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:ILE:O	1:D:398:VAL:HG13	2.22	0.40
1:D:598:ALA:O	1:D:600:ILE:HG23	2.22	0.40
1:D:628:ASP:O	1:D:631:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	661/736 (90%)	578 (87%)	69 (10%)	14 (2%)	5	31
1	B	661/736 (90%)	578 (87%)	68 (10%)	15 (2%)	5	29
1	C	661/736 (90%)	578 (87%)	69 (10%)	14 (2%)	5	31
1	D	661/736 (90%)	579 (88%)	68 (10%)	14 (2%)	5	31
All	All	2644/2944 (90%)	2313 (88%)	274 (10%)	57 (2%)	5	29

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	PRO
1	A	662	ARG
1	B	224	PRO
1	C	224	PRO
1	C	662	ARG
1	D	224	PRO
1	D	662	ARG
1	A	129	GLY
1	A	618	ILE
1	A	658	HIS
1	B	129	GLY
1	B	618	ILE

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Mol	Chain	Res	Type
1	B	658	HIS
1	B	662	ARG
1	C	129	GLY
1	C	618	ILE
1	C	658	HIS
1	D	129	GLY
1	D	618	ILE
1	D	658	HIS
1	A	389	ALA
1	B	389	ALA
1	C	389	ALA
1	D	389	ALA
1	A	76	PRO
1	A	499	VAL
1	B	76	PRO
1	B	499	VAL
1	B	628	ASP
1	C	76	PRO
1	C	499	VAL
1	D	76	PRO
1	D	499	VAL
1	D	628	ASP
1	A	143	THR
1	A	628	ASP
1	B	113	GLY
1	B	143	THR
1	C	628	ASP
1	D	143	THR
1	A	113	GLY
1	A	177	PHE
1	B	177	PHE
1	B	703	LEU
1	C	113	GLY
1	C	143	THR
1	C	177	PHE
1	D	113	GLY
1	D	177	PHE
1	A	484	VAL
1	B	183	VAL
1	B	484	VAL
1	C	183	VAL
1	C	484	VAL

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Mol	Chain	Res	Type
1	D	183	VAL
1	D	484	VAL
1	A	183	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	523/586 (89%)	481 (92%)	42 (8%)	11	40
1	B	523/586 (89%)	480 (92%)	43 (8%)	10	39
1	C	523/586 (89%)	480 (92%)	43 (8%)	10	39
1	D	523/586 (89%)	480 (92%)	43 (8%)	10	39
All	All	2092/2344 (89%)	1921 (92%)	171 (8%)	10	39

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	109	ILE
1	A	150	THR
1	A	164	MET
1	A	165	VAL
1	A	172	VAL
1	A	183	VAL
1	A	184	VAL
1	A	193	VAL
1	A	219	LEU
1	A	220	LEU
1	A	250	LEU
1	A	252	VAL
1	A	264	VAL
1	A	277	THR
1	A	307	LEU
1	A	319	VAL
1	A	322	VAL

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Mol	Chain	Res	Type
1	A	344	VAL
1	A	367	LEU
1	A	382	CYS
1	A	386	LEU
1	A	424	VAL
1	A	442	VAL
1	A	443	THR
1	A	458	LEU
1	A	466	LEU
1	A	479	LEU
1	A	504	VAL
1	A	506	ILE
1	A	536	VAL
1	A	562	THR
1	A	583	THR
1	A	596	VAL
1	A	645	THR
1	A	647	VAL
1	A	674	THR
1	A	693	VAL
1	A	707	LEU
1	A	708	LEU
1	A	712	ILE
1	A	726	ILE
1	B	105	LEU
1	B	109	ILE
1	B	150	THR
1	B	164	MET
1	B	165	VAL
1	B	172	VAL
1	B	183	VAL
1	B	184	VAL
1	B	193	VAL
1	B	219	LEU
1	B	220	LEU
1	B	250	LEU
1	B	252	VAL
1	B	264	VAL
1	B	277	THR
1	B	307	LEU
1	B	319	VAL
1	B	322	VAL

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Mol	Chain	Res	Type
1	B	344	VAL
1	B	367	LEU
1	B	382	CYS
1	B	386	LEU
1	B	424	VAL
1	B	438	LEU
1	B	442	VAL
1	B	443	THR
1	B	458	LEU
1	B	466	LEU
1	B	479	LEU
1	B	504	VAL
1	B	506	ILE
1	B	536	VAL
1	B	562	THR
1	B	583	THR
1	B	596	VAL
1	B	645	THR
1	B	647	VAL
1	B	674	THR
1	B	693	VAL
1	B	707	LEU
1	B	708	LEU
1	B	712	ILE
1	B	726	ILE
1	C	105	LEU
1	C	109	ILE
1	C	150	THR
1	C	164	MET
1	C	165	VAL
1	C	172	VAL
1	C	183	VAL
1	C	184	VAL
1	C	193	VAL
1	C	219	LEU
1	C	220	LEU
1	C	250	LEU
1	C	252	VAL
1	C	264	VAL
1	C	277	THR
1	C	307	LEU
1	C	319	VAL

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Mol	Chain	Res	Type
1	C	322	VAL
1	C	344	VAL
1	C	367	LEU
1	C	382	CYS
1	C	386	LEU
1	C	424	VAL
1	C	438	LEU
1	C	442	VAL
1	C	443	THR
1	C	458	LEU
1	C	466	LEU
1	C	479	LEU
1	C	504	VAL
1	C	506	ILE
1	C	536	VAL
1	C	562	THR
1	C	583	THR
1	C	596	VAL
1	C	645	THR
1	C	647	VAL
1	C	674	THR
1	C	693	VAL
1	C	707	LEU
1	C	708	LEU
1	C	712	ILE
1	C	726	ILE
1	D	105	LEU
1	D	109	ILE
1	D	150	THR
1	D	164	MET
1	D	165	VAL
1	D	172	VAL
1	D	183	VAL
1	D	184	VAL
1	D	193	VAL
1	D	219	LEU
1	D	220	LEU
1	D	250	LEU
1	D	252	VAL
1	D	264	VAL
1	D	277	THR
1	D	307	LEU

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Mol	Chain	Res	Type
1	D	319	VAL
1	D	322	VAL
1	D	344	VAL
1	D	367	LEU
1	D	382	CYS
1	D	386	LEU
1	D	424	VAL
1	D	442	VAL
1	D	443	THR
1	D	458	LEU
1	D	466	LEU
1	D	479	LEU
1	D	504	VAL
1	D	506	ILE
1	D	536	VAL
1	D	562	THR
1	D	574	VAL
1	D	583	THR
1	D	596	VAL
1	D	645	THR
1	D	647	VAL
1	D	674	THR
1	D	693	VAL
1	D	707	LEU
1	D	708	LEU
1	D	712	ILE
1	D	726	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	HIS
1	A	498	GLN
1	A	567	GLN
1	B	308	HIS
1	B	450	ASN
1	B	498	GLN
1	B	502	HIS
1	B	513	GLN
1	B	567	GLN
1	C	308	HIS
1	C	567	GLN

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Mol	Chain	Res	Type
1	D	112	ASN
1	D	308	HIS
1	D	513	GLN
1	D	567	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	ALF	A	995	-	4,4,4	1.35	0	-		
2	ALF	B	995	-	4,4,4	1.37	0	-		
2	ALF	D	995	-	4,4,4	1.37	0	-		
2	ALF	C	995	-	4,4,4	1.35	0	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	995	ALF	2	0
2	D	995	ALF	1	0
2	C	995	ALF	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	663/736 (90%)	-0.07	11 (1%)	69 49	56, 106, 243, 371	0
1	B	663/736 (90%)	-0.05	14 (2%)	63 43	55, 106, 244, 373	0
1	C	663/736 (90%)	-0.04	15 (2%)	61 41	55, 106, 244, 371	0
1	D	663/736 (90%)	-0.07	9 (1%)	73 54	56, 106, 244, 369	0
All	All	2652/2944 (90%)	-0.06	49 (1%)	67 48	55, 106, 244, 373	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	GLY	5.2
1	D	501	GLY	4.9
1	C	500	ASP	4.9
1	D	500	ASP	4.4
1	B	500	ASP	4.1
1	D	489	ALA	4.1
1	C	501	GLY	3.6
1	B	280	PRO	3.6
1	A	489	ALA	3.5
1	A	500	ASP	3.5
1	A	501	GLY	3.4
1	C	489	ALA	3.3
1	D	280	PRO	3.2
1	B	489	ALA	3.1
1	B	214	SER	3.0
1	C	177	PHE	2.9
1	A	280	PRO	2.9
1	C	280	PRO	2.9
1	A	177	PHE	2.8
1	A	214	SER	2.7
1	B	304	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	171	GLY	2.7
1	B	171	GLY	2.6
1	A	304	MET	2.5
1	A	278	GLY	2.5
1	C	235	SER	2.4
1	A	736	LEU	2.4
1	D	481	LEU	2.4
1	B	177	PHE	2.4
1	B	481	LEU	2.4
1	B	736	LEU	2.4
1	C	278	GLY	2.3
1	C	214	SER	2.3
1	B	235	SER	2.3
1	C	304	MET	2.2
1	D	707	LEU	2.2
1	B	636	ASP	2.2
1	D	736	LEU	2.2
1	A	636	ASP	2.2
1	D	177	PHE	2.2
1	B	278	GLY	2.1
1	C	296	ILE	2.1
1	C	481	LEU	2.1
1	D	171	GLY	2.1
1	A	235	SER	2.1
1	B	274	SER	2.1
1	C	176	ALA	2.0
1	C	250	LEU	2.0
1	C	707	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	B	997	1/1	0.79	0.17	154,154,154,154	0
4	K	C	997	1/1	0.81	0.12	144,144,144,144	0
4	K	A	997	1/1	0.83	0.14	141,141,141,141	0
4	K	D	997	1/1	0.84	0.14	160,160,160,160	0
2	ALF	D	995	5/5	0.95	0.10	57,62,80,127	0
2	ALF	B	995	5/5	0.96	0.08	48,60,80,130	0
3	MG	B	996	1/1	0.96	0.12	67,67,67,67	0
2	ALF	C	995	5/5	0.97	0.07	45,57,62,117	0
2	ALF	A	995	5/5	0.98	0.09	37,50,60,136	0
3	MG	C	996	1/1	0.98	0.12	58,58,58,58	0
3	MG	A	996	1/1	0.99	0.10	68,68,68,68	0
3	MG	D	996	1/1	0.99	0.15	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.