



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:54 AM UTC

PDB ID : 4K0J / pdb_00004k0j
Title : X-ray crystal structure of a heavy metal efflux pump, crystal form I
Authors : Pak, J.E.; Stroud, R.M.; Ngonlong Ekende, E.; Vandenbussche, G.; Center for Structures of Membrane Proteins (CSMP)
Deposited on : 2013-04-04
Resolution : 3.00 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
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

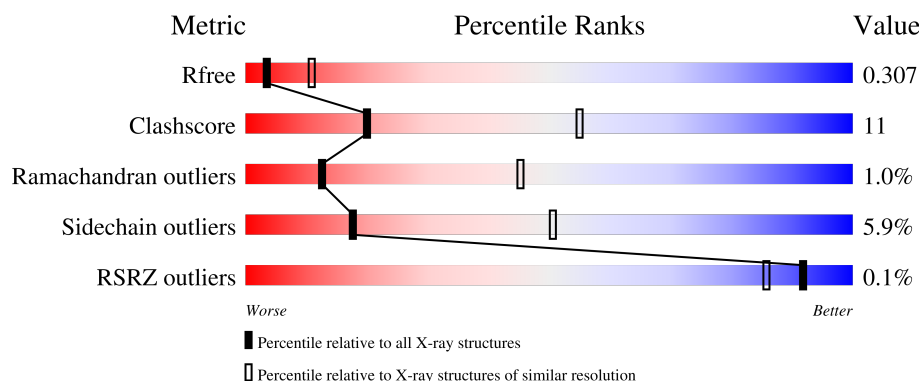
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1045	
1	B	1045	
1	C	1045	
1	D	1045	
1	E	1045	

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Mol	Chain	Length	Quality of chain
1	F	1045	61% 28% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 44018 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 Heavy metal cation tricomponent efflux pump ZneA(CzcA-like).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	958	Total	C	N	O	S	0	0	0
			7336	4709	1276	1319	32			
1	B	954	Total	C	N	O	S	0	0	0
			7314	4696	1274	1312	32			
1	C	959	Total	C	N	O	S	0	0	0
			7357	4719	1282	1324	32			
1	D	958	Total	C	N	O	S	0	0	0
			7336	4709	1276	1319	32			
1	E	954	Total	C	N	O	S	0	0	0
			7314	4696	1274	1312	32			
1	F	959	Total	C	N	O	S	0	0	0
			7357	4719	1282	1324	32			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1040	HIS	-	expression tag	UNP Q1LCD8
A	1041	HIS	-	expression tag	UNP Q1LCD8
A	1042	HIS	-	expression tag	UNP Q1LCD8
A	1043	HIS	-	expression tag	UNP Q1LCD8
A	1044	HIS	-	expression tag	UNP Q1LCD8
A	1045	HIS	-	expression tag	UNP Q1LCD8
B	1040	HIS	-	expression tag	UNP Q1LCD8
B	1041	HIS	-	expression tag	UNP Q1LCD8
B	1042	HIS	-	expression tag	UNP Q1LCD8
B	1043	HIS	-	expression tag	UNP Q1LCD8
B	1044	HIS	-	expression tag	UNP Q1LCD8
B	1045	HIS	-	expression tag	UNP Q1LCD8
C	1040	HIS	-	expression tag	UNP Q1LCD8
C	1041	HIS	-	expression tag	UNP Q1LCD8
C	1042	HIS	-	expression tag	UNP Q1LCD8
C	1043	HIS	-	expression tag	UNP Q1LCD8
C	1044	HIS	-	expression tag	UNP Q1LCD8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1045	HIS	-	expression tag	UNP Q1LCD8
D	1040	HIS	-	expression tag	UNP Q1LCD8
D	1041	HIS	-	expression tag	UNP Q1LCD8
D	1042	HIS	-	expression tag	UNP Q1LCD8
D	1043	HIS	-	expression tag	UNP Q1LCD8
D	1044	HIS	-	expression tag	UNP Q1LCD8
D	1045	HIS	-	expression tag	UNP Q1LCD8
E	1040	HIS	-	expression tag	UNP Q1LCD8
E	1041	HIS	-	expression tag	UNP Q1LCD8
E	1042	HIS	-	expression tag	UNP Q1LCD8
E	1043	HIS	-	expression tag	UNP Q1LCD8
E	1044	HIS	-	expression tag	UNP Q1LCD8
E	1045	HIS	-	expression tag	UNP Q1LCD8
F	1040	HIS	-	expression tag	UNP Q1LCD8
F	1041	HIS	-	expression tag	UNP Q1LCD8
F	1042	HIS	-	expression tag	UNP Q1LCD8
F	1043	HIS	-	expression tag	UNP Q1LCD8
F	1044	HIS	-	expression tag	UNP Q1LCD8
F	1045	HIS	-	expression tag	UNP Q1LCD8

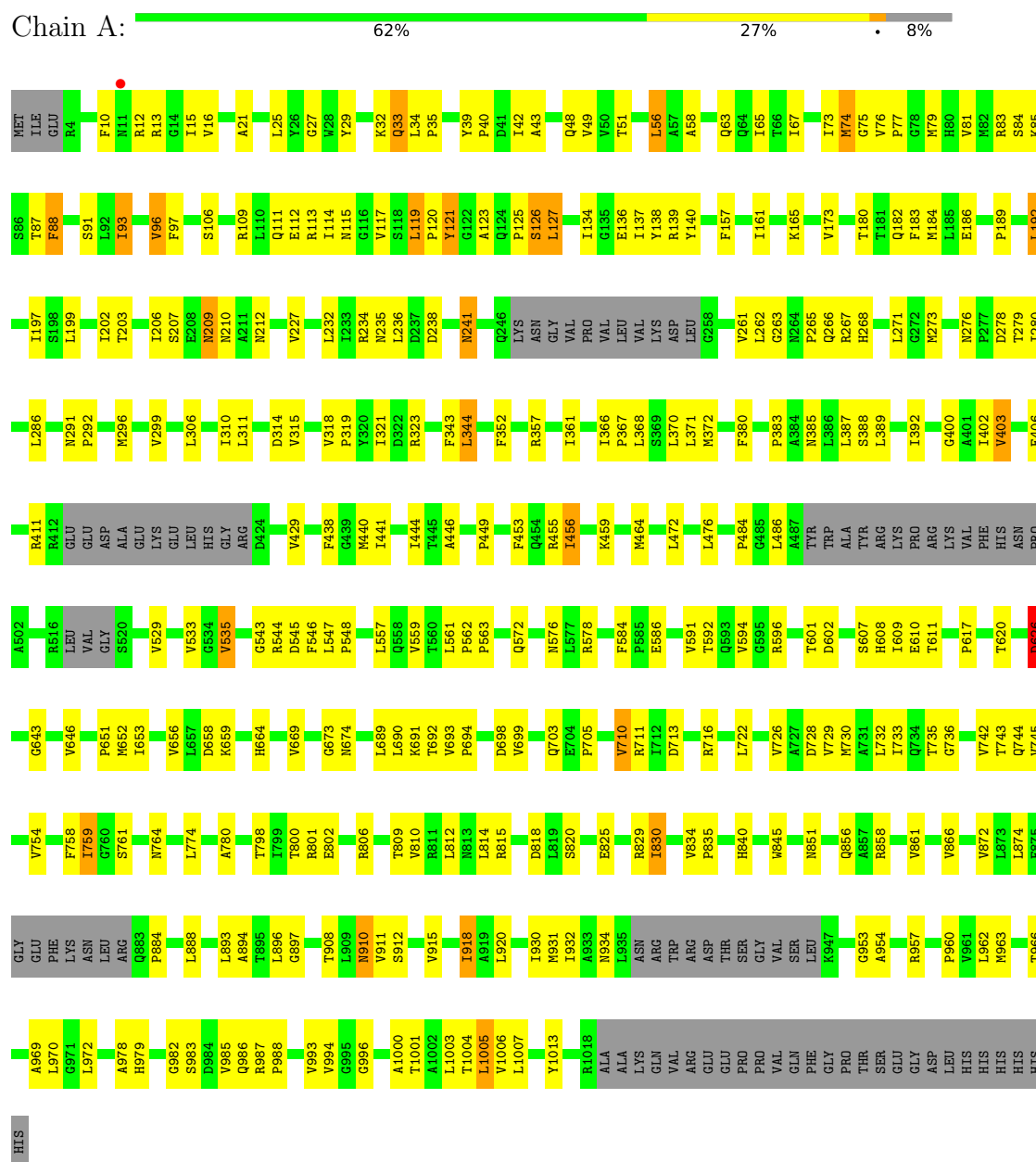
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0

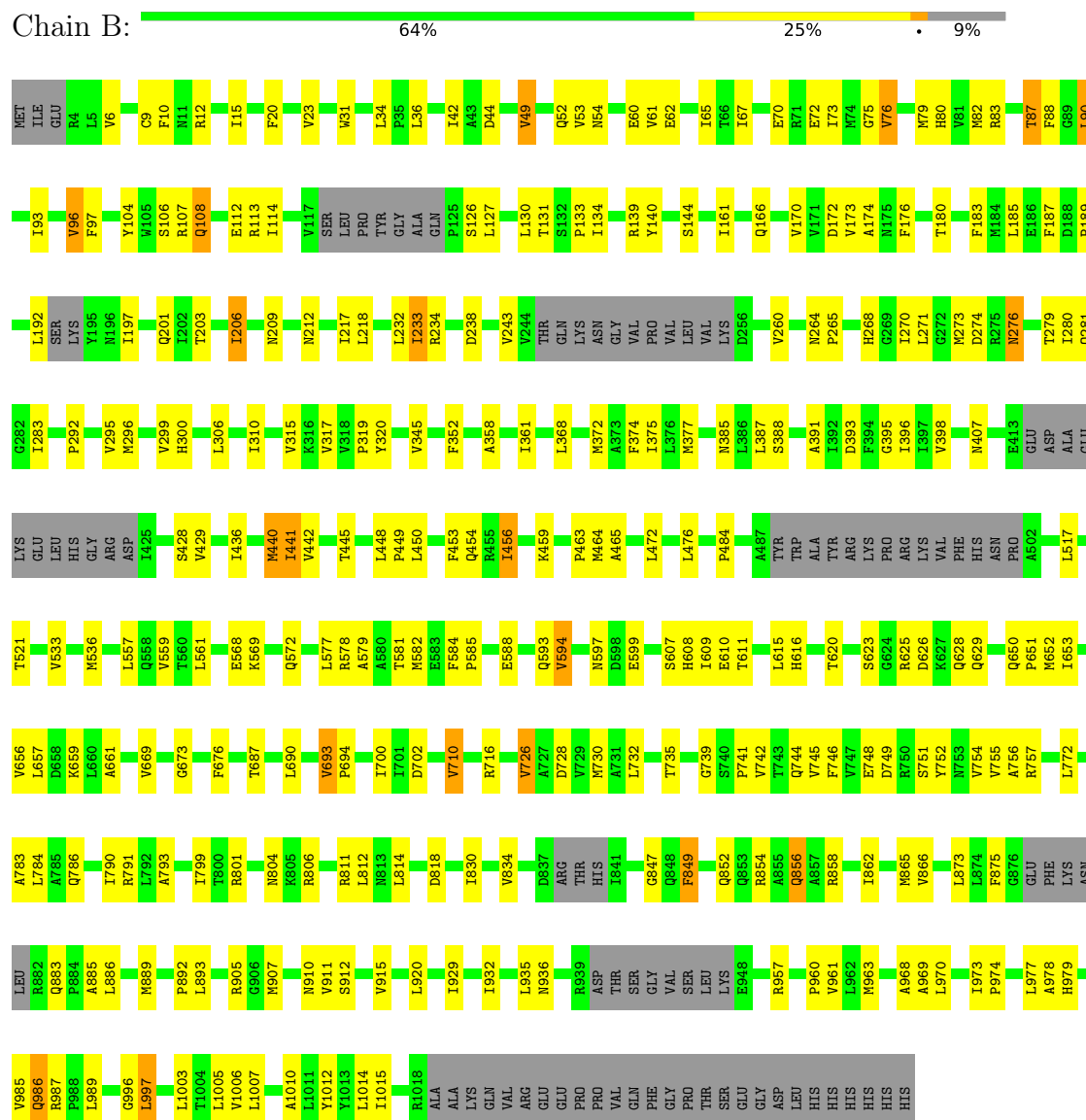
3 Residue-property plots

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

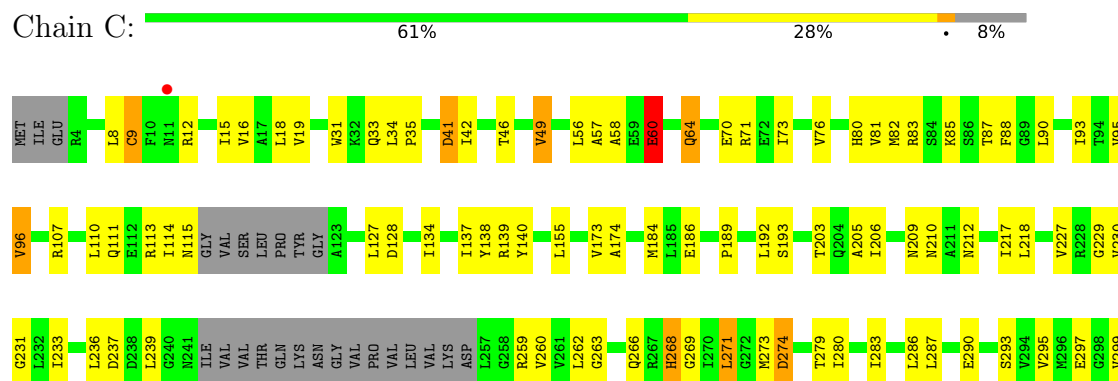
- Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)

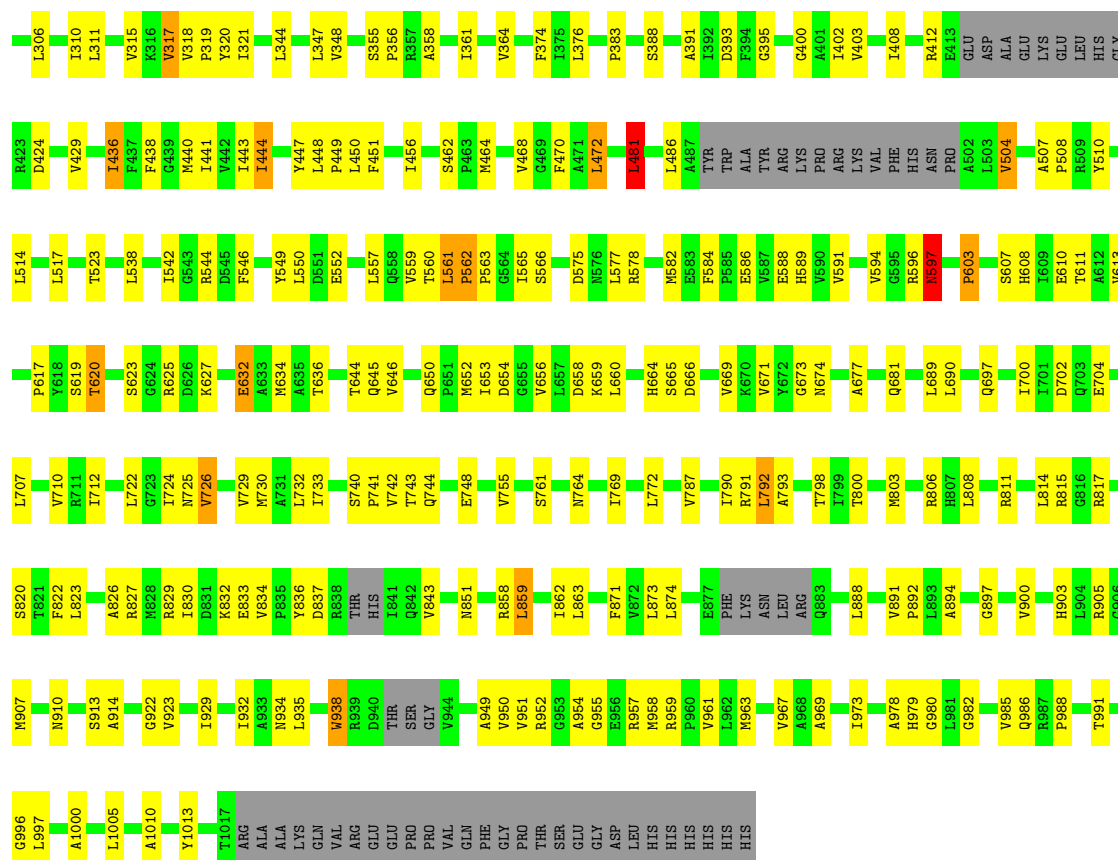


• Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)



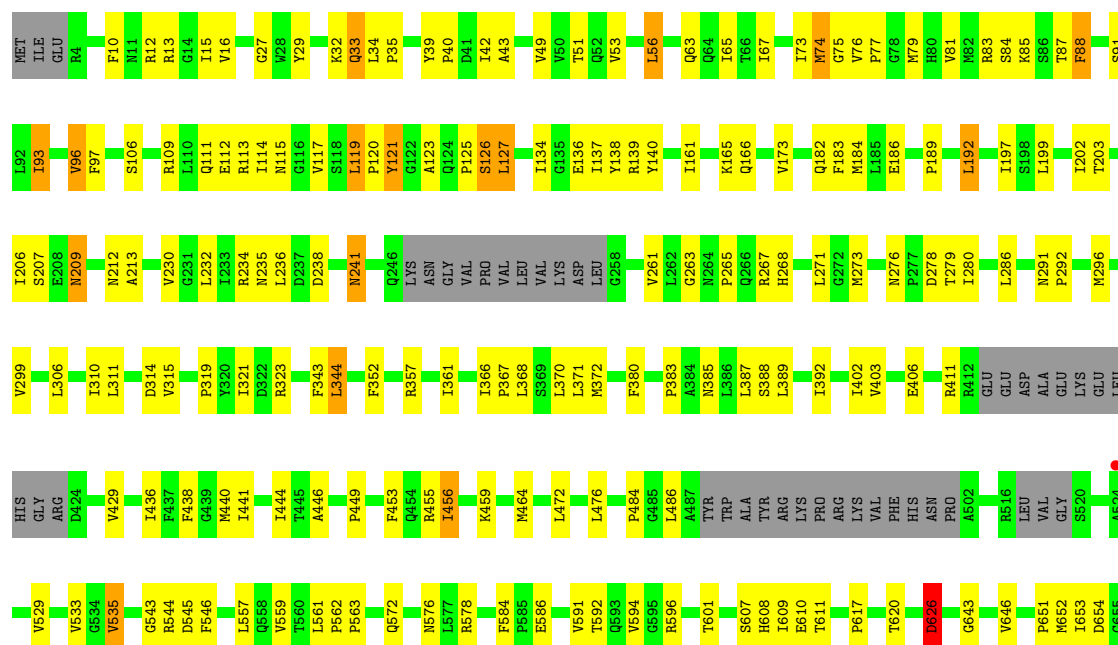
• Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)

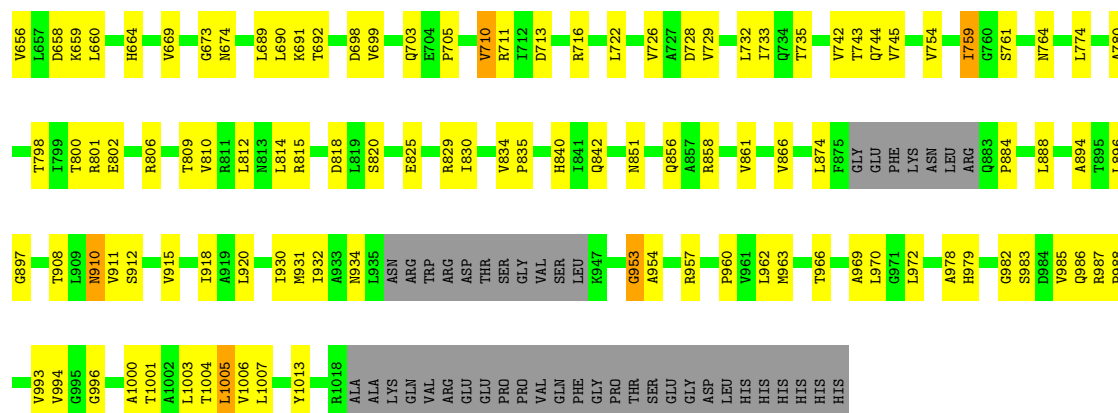




- Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)

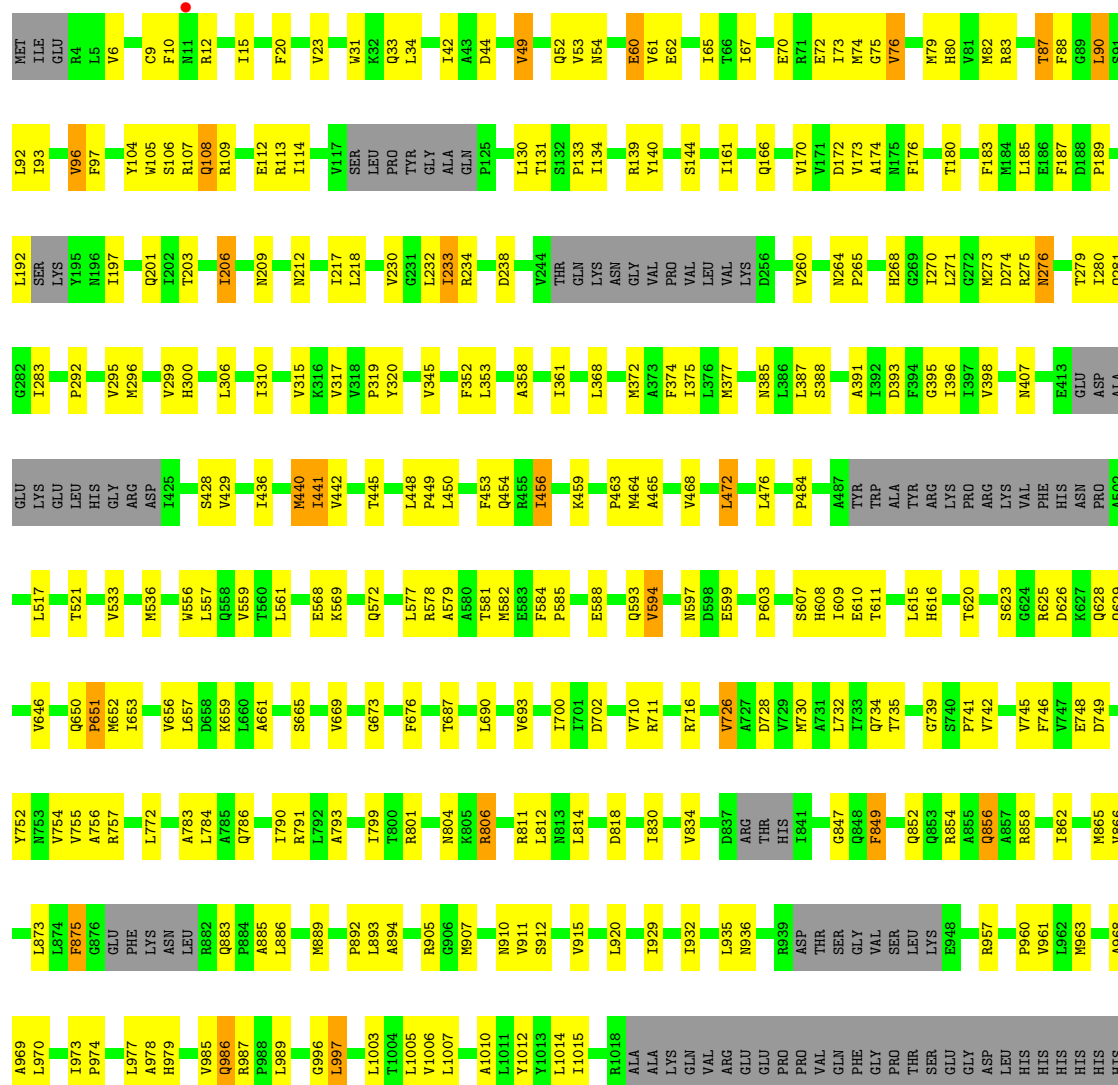
Chain D: 64% 26% 8%





- Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)

Chain E: 63% 26% 9%



- Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.63Å 129.06Å 392.37Å 90.00° 94.62° 90.00°	Depositor
Resolution (Å)	19.98 – 3.00 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.98-3.00) 85.2 (19.98-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.279 , 0.305 0.280 , 0.307	Depositor DCC
R_{free} test set	1925 reflections (0.88%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	44018	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: ZN

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	0/7461	0.80	6/10149 (0.1%)
1	B	0.36	0/7436	0.82	4/10111 (0.0%)
1	C	0.36	0/7480	0.83	9/10170 (0.1%)
1	D	0.35	0/7461	0.80	3/10149 (0.0%)
1	E	0.36	0/7436	0.81	4/10111 (0.0%)
1	F	0.36	0/7480	0.82	6/10170 (0.1%)
All	All	0.36	0/44754	0.81	32/60860 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	538	LEU	N-CA-C	-7.16	106.46	114.62
1	C	538	LEU	N-CA-C	-7.14	106.47	114.62
1	C	90	LEU	N-CA-C	7.11	118.95	108.14
1	F	90	LEU	N-CA-C	6.90	118.63	108.14
1	A	830	ILE	N-CA-C	6.10	116.58	110.23
1	E	90	LEU	N-CA-C	6.09	117.80	108.42
1	D	830	ILE	N-CA-C	6.07	116.54	110.23
1	D	119	LEU	CA-C-N	6.04	127.39	119.84
1	D	119	LEU	C-N-CA	6.04	127.39	119.84
1	B	90	LEU	N-CA-C	5.96	117.91	108.79
1	F	60	GLU	N-CA-C	-5.91	106.70	112.97
1	A	119	LEU	CA-C-N	5.90	127.22	119.84
1	A	119	LEU	C-N-CA	5.90	127.22	119.84
1	C	60	GLU	N-CA-C	-5.79	106.83	112.97
1	F	597	ASN	N-CA-C	5.74	114.26	108.75
1	C	597	ASN	N-CA-C	5.57	114.09	108.75
1	B	693	VAL	CA-C-N	5.46	125.80	119.47
1	B	693	VAL	C-N-CA	5.46	125.80	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	693	VAL	CA-C-N	5.41	125.75	119.47
1	E	693	VAL	C-N-CA	5.41	125.75	119.47
1	F	748	GLU	CB-CA-C	-5.38	110.39	116.63
1	C	748	GLU	CB-CA-C	-5.34	110.43	116.63
1	F	58	ALA	N-CA-C	5.20	118.44	112.57
1	C	562	PRO	CA-C-N	5.15	124.91	119.76
1	C	562	PRO	C-N-CA	5.15	124.91	119.76
1	C	646	VAL	N-CA-C	5.15	115.27	107.75
1	A	602	ASP	CA-C-N	5.13	126.96	121.00
1	A	602	ASP	C-N-CA	5.13	126.96	121.00
1	C	58	ALA	N-CA-C	5.12	118.35	112.57
1	E	748	GLU	CB-CA-C	-5.10	110.71	116.63
1	A	58	ALA	N-CA-C	5.09	117.22	111.11
1	B	748	GLU	CB-CA-C	-5.04	110.79	116.63

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	7336	0	7607	175	0
1	B	7314	0	7588	164	0
1	C	7357	0	7626	184	0
1	D	7336	0	7607	165	0
1	E	7314	0	7588	175	0
1	F	7357	0	7626	189	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
All	All	44018	0	45642	1019	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 11.

All (1019) 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:D:388:SER:HB2	1:D:464:MET:HB2	1.60	0.83
1:D:429:VAL:HG21	1:D:484:PRO:HB3	1.61	0.82
1:A:388:SER:HB2	1:A:464:MET:HB2	1.61	0.81
1:A:429:VAL:HG21	1:A:484:PRO:HB3	1.62	0.81
1:D:544:ARG:HH22	1:D:856:GLN:HG2	1.50	0.77
1:A:544:ARG:HH22	1:A:856:GLN:HG2	1.51	0.75
1:E:83:ARG:NH2	1:E:659:LYS:O	2.20	0.75
1:D:934:ASN:HD22	1:D:957:ARG:HB2	1.52	0.74
1:D:111:GLN:O	1:D:115:ASN:ND2	2.20	0.74
1:A:934:ASN:HD22	1:A:957:ARG:HB2	1.52	0.74
1:D:138:TYR:HB2	1:D:296:MET:HE1	1.70	0.73
1:F:12:ARG:HG2	1:F:15:ILE:HB	1.69	0.73
1:A:111:GLN:O	1:A:115:ASN:ND2	2.19	0.73
1:B:83:ARG:NH2	1:B:659:LYS:O	2.21	0.73
1:A:138:TYR:HB2	1:A:296:MET:HE1	1.68	0.73
1:B:62:GLU:OE1	1:B:801:ARG:NH1	2.22	0.72
1:E:559:VAL:HB	1:E:609:ILE:HB	1.70	0.72
1:C:12:ARG:HG2	1:C:15:ILE:HB	1.69	0.72
1:D:119:LEU:HD12	1:D:125:PRO:HD3	1.72	0.72
1:E:107:ARG:HD3	1:E:130:LEU:HD13	1.72	0.72
1:B:107:ARG:HD3	1:B:130:LEU:HD13	1.70	0.71
1:D:134:ILE:HG22	1:D:652:MET:HB3	1.71	0.71
1:F:70:GLU:HA	1:F:82:MET:HE1	1.73	0.71
1:B:559:VAL:HB	1:B:609:ILE:HB	1.70	0.71
1:E:233:ILE:HG13	1:E:238:ASP:HB2	1.72	0.71
1:A:134:ILE:HG22	1:A:652:MET:HB3	1.73	0.71
1:A:119:LEU:HD12	1:A:125:PRO:HD3	1.72	0.70
1:E:62:GLU:OE1	1:E:801:ARG:NH1	2.24	0.70
1:C:111:GLN:O	1:C:115:ASN:ND2	2.23	0.70
1:E:407:ASN:ND2	1:E:428:SER:OG	2.24	0.70
1:B:233:ILE:HG13	1:B:238:ASP:HB2	1.72	0.70
1:B:936:ASN:ND2	1:B:1012:TYR:OH	2.24	0.70
1:C:70:GLU:HA	1:C:82:MET:HE1	1.73	0.70
1:B:407:ASN:ND2	1:B:428:SER:OG	2.25	0.70
1:D:453:PHE:HA	1:D:858:ARG:HD2	1.73	0.70
1:E:936:ASN:ND2	1:E:1012:TYR:OH	2.24	0.69
1:D:535:VAL:HG12	1:D:896:LEU:HB2	1.73	0.69
1:A:453:PHE:HA	1:A:858:ARG:HD2	1.73	0.69
1:A:535:VAL:HG12	1:A:896:LEU:HB2	1.73	0.69
1:F:111:GLN:O	1:F:115:ASN:ND2	2.25	0.69
1:F:205:ALA:O	1:F:209:ASN:ND2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:533:VAL:HA	1:E:536:MET:HE2	1.75	0.69
1:C:361:ILE:HB	1:C:486:LEU:HD13	1.74	0.68
1:F:361:ILE:HB	1:F:486:LEU:HD13	1.74	0.68
1:C:205:ALA:O	1:C:209:ASN:ND2	2.25	0.68
1:D:559:VAL:HB	1:D:609:ILE:HB	1.76	0.68
1:B:42:ILE:HG23	1:B:456:ILE:HB	1.76	0.68
1:B:72:GLU:O	1:B:113:ARG:NH1	2.27	0.68
1:A:559:VAL:HB	1:A:609:ILE:HB	1.76	0.67
1:D:271:LEU:HD23	1:D:279:THR:HG23	1.75	0.67
1:C:650:GLN:HB2	1:C:653:ILE:HG22	1.77	0.67
1:D:81:VAL:HB	1:D:96:VAL:HG13	1.77	0.67
1:A:81:VAL:HB	1:A:96:VAL:HG13	1.76	0.67
1:A:271:LEU:HD23	1:A:279:THR:HG23	1.76	0.67
1:E:72:GLU:O	1:E:113:ARG:NH1	2.27	0.66
1:B:533:VAL:HA	1:B:536:MET:HE2	1.76	0.66
1:E:42:ILE:HG23	1:E:456:ILE:HB	1.76	0.66
1:F:650:GLN:HB2	1:F:653:ILE:HG22	1.76	0.66
1:C:388:SER:HB2	1:C:464:MET:HB2	1.78	0.66
1:E:12:ARG:HG2	1:E:15:ILE:HB	1.78	0.66
1:F:597:ASN:OD1	1:F:597:ASN:N	2.30	0.65
1:F:139:ARG:HD2	1:F:321:ILE:HD12	1.78	0.65
1:F:388:SER:HB2	1:F:464:MET:HB2	1.77	0.65
1:B:12:ARG:HG2	1:B:15:ILE:HB	1.78	0.65
1:E:271:LEU:HD22	1:E:281:GLN:HB3	1.78	0.65
1:F:549:TYR:OH	1:F:627:LYS:NZ	2.30	0.65
1:A:306:LEU:HD23	1:A:310:ILE:HB	1.78	0.65
1:D:12:ARG:HG2	1:D:15:ILE:HD12	1.79	0.65
1:C:443:ILE:HG13	1:C:922:GLY:HA3	1.79	0.65
1:D:711:ARG:NH1	1:D:713:ASP:OD2	2.30	0.64
1:F:443:ILE:HG13	1:F:922:GLY:HA3	1.79	0.64
1:C:597:ASN:N	1:C:597:ASN:OD1	2.30	0.64
1:D:306:LEU:HD23	1:D:310:ILE:HB	1.80	0.64
1:A:206:ILE:HG23	1:A:742:VAL:HG11	1.80	0.64
1:B:212:ASN:ND2	1:C:60:GLU:OE2	2.31	0.64
1:D:27:GLY:HA3	1:D:371:LEU:HB3	1.80	0.64
1:F:110:LEU:HD23	1:F:127:LEU:HD11	1.80	0.64
1:C:549:TYR:OH	1:C:627:LYS:NZ	2.29	0.64
1:C:110:LEU:HD23	1:C:127:LEU:HD11	1.78	0.64
1:D:206:ILE:HG23	1:D:742:VAL:HG11	1.80	0.64
1:E:352:PHE:HB3	1:E:963:MET:HE2	1.80	0.64
1:B:352:PHE:HB3	1:B:963:MET:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:ASN:ND2	1:F:60:GLU:OE2	2.31	0.63
1:A:962:LEU:O	1:A:966:THR:OG1	2.16	0.63
1:B:271:LEU:HD22	1:B:281:GLN:HB3	1.80	0.63
1:D:962:LEU:O	1:D:966:THR:OG1	2.16	0.63
1:B:271:LEU:HD23	1:B:279:THR:HG23	1.79	0.63
1:E:905:ARG:HB2	1:E:907:MET:HG3	1.81	0.63
1:A:674:ASN:O	1:A:806:ARG:NH2	2.31	0.63
1:D:12:ARG:HB3	1:D:16:VAL:HG13	1.80	0.63
1:E:271:LEU:HD23	1:E:279:THR:HG23	1.80	0.63
1:A:12:ARG:HB3	1:A:16:VAL:HG13	1.80	0.63
1:B:579:ALA:HA	1:B:582:MET:HE2	1.81	0.63
1:D:674:ASN:O	1:D:806:ARG:NH2	2.32	0.63
1:B:905:ARG:HB2	1:B:907:MET:HG3	1.81	0.63
1:C:557:LEU:HB2	1:C:611:THR:HB	1.81	0.62
1:E:218:LEU:HD11	1:F:769:ILE:HD11	1.81	0.62
1:A:12:ARG:HG2	1:A:15:ILE:HD12	1.79	0.62
1:A:27:GLY:HA3	1:A:371:LEU:HB3	1.80	0.62
1:C:203:THR:HA	1:C:206:ILE:HG22	1.81	0.62
1:F:203:THR:HA	1:F:206:ILE:HG22	1.82	0.62
1:F:544:ARG:HB2	1:F:820:SER:HB3	1.81	0.62
1:F:557:LEU:HB2	1:F:611:THR:HB	1.82	0.62
1:C:544:ARG:HB2	1:C:820:SER:HB3	1.82	0.62
1:D:203:THR:HG21	1:D:735:THR:HG21	1.82	0.62
1:C:139:ARG:HD2	1:C:321:ILE:HD12	1.81	0.62
1:B:232:LEU:HD23	1:B:234:ARG:HH12	1.66	0.61
1:C:608:HIS:HE1	1:C:610:GLU:HG3	1.65	0.61
1:D:626:ASP:OD1	1:D:626:ASP:N	2.33	0.61
1:F:306:LEU:HD23	1:F:310:ILE:HD12	1.82	0.61
1:A:626:ASP:N	1:A:626:ASP:OD1	2.33	0.61
1:B:716:ARG:HE	1:B:726:VAL:HG11	1.65	0.61
1:D:76:VAL:HG12	1:D:113:ARG:HG3	1.82	0.61
1:A:136:GLU:OE1	1:A:139:ARG:NH2	2.33	0.61
1:A:203:THR:HG21	1:A:735:THR:HG21	1.82	0.61
1:B:218:LEU:HD11	1:C:769:ILE:HD11	1.82	0.61
1:E:387:LEU:HB3	1:E:985:VAL:HG11	1.82	0.61
1:B:702:ASP:OD1	1:B:811:ARG:NH1	2.34	0.61
1:E:579:ALA:HA	1:E:582:MET:HE2	1.83	0.61
1:E:716:ARG:HE	1:E:726:VAL:HG11	1.65	0.61
1:F:83:ARG:NH2	1:F:658:ASP:O	2.34	0.61
1:A:76:VAL:HG12	1:A:113:ARG:HG3	1.83	0.61
1:A:711:ARG:NH1	1:A:713:ASP:OD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:ILE:HD11	1:F:239:LEU:HD11	1.83	0.60
1:B:561:LEU:HB2	1:B:607:SER:O	2.00	0.60
1:C:206:ILE:HD11	1:C:239:LEU:HD11	1.83	0.60
1:C:897:GLY:HA2	1:C:900:VAL:HG22	1.82	0.60
1:C:85:LYS:HG3	1:C:800:THR:HG22	1.83	0.60
1:F:961:VAL:HG11	1:F:1005:LEU:HD21	1.83	0.60
1:C:184:MET:HE2	1:C:263:GLY:HA3	1.83	0.60
1:C:306:LEU:HD23	1:C:310:ILE:HD12	1.84	0.60
1:F:49:VAL:HG13	1:F:93:ILE:HB	1.84	0.60
1:F:233:ILE:HD11	1:F:239:LEU:HB2	1.83	0.60
1:A:983:SER:OG	1:A:987:ARG:NH2	2.35	0.60
1:D:63:GLN:HA	1:D:67:ILE:HD12	1.84	0.60
1:F:608:HIS:HE1	1:F:610:GLU:HG3	1.67	0.60
1:C:83:ARG:NH2	1:C:658:ASP:O	2.35	0.60
1:F:85:LYS:HG3	1:F:800:THR:HG22	1.84	0.60
1:A:63:GLN:HA	1:A:67:ILE:HD12	1.84	0.59
1:D:136:GLU:OE1	1:D:139:ARG:NH2	2.34	0.59
1:E:561:LEU:HB2	1:E:607:SER:O	2.02	0.59
1:C:49:VAL:HG13	1:C:93:ILE:HB	1.85	0.59
1:D:983:SER:OG	1:D:987:ARG:NH2	2.35	0.59
1:C:761:SER:HA	1:C:764:ASN:HD22	1.67	0.59
1:B:76:VAL:HG23	1:B:79:MET:HB2	1.85	0.59
1:B:387:LEU:HB3	1:B:985:VAL:HG11	1.83	0.59
1:C:961:VAL:HG11	1:C:1005:LEU:HD21	1.83	0.59
1:D:74:MET:HA	1:D:79:MET:HE1	1.85	0.59
1:E:456:ILE:HA	1:E:459:LYS:HD2	1.84	0.59
1:A:563:PRO:HB3	1:A:705:PRO:HD2	1.83	0.59
1:F:897:GLY:HA2	1:F:900:VAL:HG22	1.83	0.59
1:E:232:LEU:HD23	1:E:234:ARG:HH12	1.67	0.59
1:F:905:ARG:NH2	1:F:991:THR:OG1	2.32	0.59
1:B:52:GLN:NE2	1:B:599:GLU:O	2.35	0.59
1:E:440:MET:HG2	1:E:476:LEU:HD22	1.85	0.59
1:E:801:ARG:NH2	1:E:804:ASN:OD1	2.36	0.59
1:F:184:MET:HE2	1:F:263:GLY:HA3	1.83	0.59
1:F:273:MET:HG3	1:F:591:VAL:HG22	1.85	0.59
1:D:456:ILE:HA	1:D:459:LYS:HD2	1.85	0.59
1:E:52:GLN:NE2	1:E:599:GLU:O	2.35	0.58
1:A:931:MET:HE1	1:A:954:ALA:HA	1.84	0.58
1:B:456:ILE:HA	1:B:459:LYS:HD2	1.84	0.58
1:E:985:VAL:HG13	1:E:986:GLN:HG3	1.84	0.58
1:D:982:GLY:O	1:D:986:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:MET:HG2	1:B:476:LEU:HD22	1.84	0.58
1:B:985:VAL:HG13	1:B:986:GLN:HG3	1.86	0.58
1:C:271:LEU:HD23	1:C:279:THR:HG23	1.85	0.58
1:A:235:ASN:ND2	1:A:238:ASP:OD1	2.36	0.58
1:A:703:GLN:HE22	1:A:809:THR:H	1.52	0.58
1:A:982:GLY:O	1:A:986:GLN:NE2	2.36	0.58
1:A:456:ILE:HA	1:A:459:LYS:HD2	1.85	0.58
1:C:982:GLY:O	1:C:986:GLN:NE2	2.36	0.58
1:D:931:MET:HE1	1:D:954:ALA:HA	1.84	0.58
1:E:702:ASP:OD1	1:E:811:ARG:NH1	2.36	0.58
1:C:233:ILE:HD11	1:C:239:LEU:HB2	1.85	0.58
1:C:273:MET:HG3	1:C:591:VAL:HG22	1.86	0.58
1:D:703:GLN:HE22	1:D:809:THR:H	1.52	0.58
1:C:608:HIS:CE1	1:C:610:GLU:HG3	2.39	0.58
1:F:761:SER:HA	1:F:764:ASN:HD22	1.68	0.58
1:B:183:PHE:HB2	1:B:754:VAL:HA	1.86	0.57
1:B:801:ARG:NH2	1:B:804:ASN:OD1	2.37	0.57
1:A:535:VAL:HA	1:A:896:LEU:HD13	1.85	0.57
1:B:912:SER:OG	1:B:985:VAL:O	2.22	0.57
1:F:730:MET:HA	1:F:733:ILE:HD12	1.86	0.57
1:C:905:ARG:NH2	1:C:991:THR:OG1	2.31	0.57
1:D:209:ASN:HB2	1:E:726:VAL:HG13	1.85	0.57
1:D:273:MET:O	1:D:578:ARG:NE	2.35	0.57
1:A:74:MET:HA	1:A:79:MET:HE1	1.86	0.57
1:B:44:ASP:OD1	1:B:459:LYS:NZ	2.37	0.57
1:F:271:LEU:HD23	1:F:279:THR:HG23	1.87	0.57
1:A:209:ASN:HB2	1:B:726:VAL:HG13	1.86	0.57
1:B:726:VAL:O	1:B:730:MET:HG2	2.05	0.57
1:F:83:ARG:NH1	1:F:660:LEU:O	2.34	0.57
1:A:343:PHE:HD2	1:A:344:LEU:HD22	1.70	0.57
1:D:557:LEU:HB2	1:D:611:THR:HB	1.87	0.57
1:B:174:ALA:HB3	1:B:283:ILE:HB	1.86	0.57
1:D:51:THR:HB	1:D:91:SER:HB3	1.85	0.57
1:F:982:GLY:O	1:F:986:GLN:NE2	2.37	0.57
1:A:557:LEU:HB2	1:A:611:THR:HB	1.87	0.56
1:A:51:THR:HB	1:A:91:SER:HB3	1.87	0.56
1:A:273:MET:O	1:A:578:ARG:NE	2.36	0.56
1:A:572:GLN:O	1:A:576:ASN:ND2	2.38	0.56
1:D:455:ARG:NH2	1:D:851:ASN:O	2.35	0.56
1:E:76:VAL:HG23	1:E:79:MET:HB2	1.86	0.56
1:E:739:GLY:HA3	1:E:757:ARG:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:791:ARG:HE	1:E:793:ALA:HB2	1.70	0.56
1:A:83:ARG:NH2	1:A:659:LYS:O	2.39	0.56
1:E:183:PHE:HB2	1:E:754:VAL:HA	1.87	0.56
1:A:273:MET:HG3	1:A:591:VAL:HG22	1.88	0.56
1:A:455:ARG:NH2	1:A:851:ASN:O	2.34	0.56
1:C:730:MET:HA	1:C:733:ILE:HD12	1.88	0.56
1:D:343:PHE:HD2	1:D:344:LEU:HD22	1.70	0.56
1:D:535:VAL:HA	1:D:896:LEU:HD13	1.86	0.56
1:A:199:LEU:HD12	1:A:732:LEU:HA	1.88	0.56
1:F:712:ILE:HG12	1:F:790:ILE:HG13	1.88	0.56
1:B:791:ARG:HE	1:B:793:ALA:HB2	1.71	0.56
1:B:739:GLY:HA3	1:B:757:ARG:HD3	1.88	0.56
1:C:712:ILE:HG12	1:C:790:ILE:HG13	1.87	0.56
1:D:199:LEU:HD12	1:D:732:LEU:HA	1.87	0.56
1:C:76:VAL:HG12	1:C:113:ARG:HG3	1.87	0.55
1:C:704:GLU:CD	1:C:704:GLU:H	2.13	0.55
1:E:140:TYR:HA	1:E:319:PRO:HA	1.88	0.55
1:E:174:ALA:HB3	1:E:283:ILE:HB	1.88	0.55
1:C:311:LEU:HD13	1:C:315:VAL:HG12	1.89	0.55
1:F:76:VAL:HG12	1:F:113:ARG:HG3	1.86	0.55
1:B:690:LEU:HD13	1:B:812:LEU:HD13	1.88	0.55
1:D:235:ASN:ND2	1:D:238:ASP:OD1	2.39	0.55
1:C:741:PRO:HA	1:C:755:VAL:HG22	1.88	0.55
1:D:189:PRO:HA	1:D:192:LEU:HB2	1.89	0.55
1:F:440:MET:HA	1:F:443:ILE:HG22	1.89	0.55
1:F:608:HIS:CE1	1:F:610:GLU:HG3	2.41	0.55
1:B:185:LEU:HD12	1:B:756:ALA:HB2	1.88	0.55
1:D:184:MET:HG3	1:D:263:GLY:HA3	1.88	0.55
1:E:690:LEU:HD13	1:E:812:LEU:HD13	1.89	0.55
1:F:311:LEU:HD13	1:F:315:VAL:HG12	1.87	0.55
1:E:276:ASN:HD21	1:E:279:THR:HB	1.71	0.55
1:F:704:GLU:H	1:F:704:GLU:CD	2.14	0.55
1:A:232:LEU:HD23	1:A:234:ARG:HH22	1.72	0.54
1:B:276:ASN:HD21	1:B:279:THR:HB	1.72	0.54
1:B:454:GLN:HB2	1:B:854:ARG:HH21	1.73	0.54
1:D:563:PRO:HB3	1:D:705:PRO:HD2	1.88	0.54
1:A:1005:LEU:HD12	1:A:1006:VAL:HG23	1.90	0.54
1:E:577:LEU:O	1:E:581:THR:OG1	2.18	0.54
1:B:279:THR:OG1	1:B:280:ILE:N	2.38	0.54
1:C:440:MET:HA	1:C:443:ILE:HG22	1.90	0.54
1:D:273:MET:HG3	1:D:591:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:912:SER:OG	1:E:985:VAL:O	2.22	0.54
1:C:702:ASP:OD1	1:C:811:ARG:NH1	2.41	0.54
1:F:891:VAL:HG23	1:F:892:PRO:HD3	1.89	0.54
1:E:279:THR:OG1	1:E:280:ILE:N	2.40	0.54
1:F:73:ILE:HD11	1:F:114:ILE:HG22	1.90	0.54
1:E:185:LEU:HD12	1:E:756:ALA:HB2	1.89	0.54
1:E:454:GLN:HB2	1:E:854:ARG:HH21	1.72	0.54
1:E:726:VAL:O	1:E:730:MET:HG2	2.08	0.54
1:D:83:ARG:NH2	1:D:659:LYS:O	2.40	0.54
1:F:741:PRO:HA	1:F:755:VAL:HG22	1.89	0.54
1:B:626:ASP:O	1:B:628:GLN:N	2.42	0.53
1:B:849:PHE:HA	1:B:852:GLN:HB3	1.90	0.53
1:D:84:SER:HB3	1:D:93:ILE:HG23	1.91	0.53
1:E:449:PRO:HB3	1:E:862:ILE:HD13	1.89	0.53
1:A:84:SER:HB3	1:A:93:ILE:HG23	1.89	0.53
1:E:858:ARG:O	1:E:862:ILE:HG13	2.09	0.53
1:F:702:ASP:OD1	1:F:811:ARG:NH1	2.41	0.53
1:E:608:HIS:HE1	1:E:610:GLU:HG3	1.74	0.53
1:F:935:LEU:HD13	1:F:954:ALA:HB2	1.91	0.53
1:A:87:THR:HB	1:A:798:THR:HG22	1.89	0.53
1:A:126:SER:OG	1:A:127:LEU:N	2.41	0.53
1:B:49:VAL:HG13	1:B:93:ILE:HB	1.90	0.53
1:B:388:SER:HB3	1:B:464:MET:HB2	1.91	0.53
1:B:577:LEU:O	1:B:581:THR:OG1	2.18	0.53
1:C:73:ILE:HD11	1:C:114:ILE:HG22	1.91	0.53
1:D:232:LEU:HD23	1:D:234:ARG:HH22	1.73	0.53
1:E:49:VAL:HG13	1:E:93:ILE:HB	1.91	0.53
1:E:388:SER:HB3	1:E:464:MET:HB2	1.91	0.53
1:B:140:TYR:HA	1:B:319:PRO:HA	1.89	0.53
1:D:1005:LEU:HD12	1:D:1006:VAL:HG23	1.91	0.53
1:A:97:PHE:CZ	1:A:106:SER:HB3	2.44	0.53
1:E:429:VAL:HG21	1:E:484:PRO:HB3	1.91	0.53
1:B:449:PRO:HB3	1:B:862:ILE:HD13	1.89	0.52
1:C:891:VAL:HG23	1:C:892:PRO:HD3	1.91	0.52
1:E:273:MET:O	1:E:578:ARG:NE	2.40	0.52
1:E:450:LEU:HD12	1:E:465:ALA:HB2	1.91	0.52
1:B:429:VAL:HG21	1:B:484:PRO:HB3	1.90	0.52
1:F:836:TYR:HB3	1:F:837:ASP:HB2	1.90	0.52
1:A:969:ALA:HB1	1:A:994:VAL:HG13	1.92	0.52
1:A:189:PRO:HA	1:A:192:LEU:HB2	1.90	0.52
1:E:97:PHE:CZ	1:E:106:SER:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:849:PHE:HA	1:E:852:GLN:HB3	1.91	0.52
1:A:119:LEU:HB3	1:A:123:ALA:HB3	1.90	0.52
1:C:935:LEU:HD13	1:C:954:ALA:HB2	1.91	0.52
1:B:597:ASN:HD22	1:B:599:GLU:H	1.56	0.52
1:E:517:LEU:HB3	1:E:1010:ALA:HB2	1.91	0.52
1:D:87:THR:OG1	1:D:88:PHE:N	2.42	0.52
1:A:43:ALA:HB2	1:A:656:VAL:HG12	1.92	0.52
1:B:517:LEU:HB3	1:B:1010:ALA:HB2	1.92	0.52
1:B:608:HIS:HE1	1:B:610:GLU:HG3	1.75	0.52
1:C:817:ARG:HH11	1:C:822:PHE:HA	1.75	0.52
1:D:559:VAL:HG22	1:D:646:VAL:HG22	1.92	0.52
1:E:44:ASP:OD1	1:E:459:LYS:NZ	2.38	0.52
1:A:733:ILE:HD13	1:C:229:GLY:HA3	1.92	0.52
1:B:450:LEU:HD12	1:B:465:ALA:HB2	1.92	0.52
1:C:9:CYS:HB2	1:C:481:LEU:HD23	1.91	0.52
1:E:449:PRO:HD3	1:E:866:VAL:HG11	1.92	0.52
1:B:97:PHE:CZ	1:B:106:SER:HB2	2.44	0.51
1:B:273:MET:HG3	1:B:274:ASP:H	1.73	0.51
1:C:83:ARG:NH1	1:C:660:LEU:O	2.33	0.51
1:D:119:LEU:HB3	1:D:123:ALA:HB3	1.91	0.51
1:D:126:SER:OG	1:D:127:LEU:N	2.38	0.51
1:E:626:ASP:O	1:E:628:GLN:N	2.42	0.51
1:F:82:MET:HG3	1:F:95:VAL:HG22	1.93	0.51
1:F:949:ALA:HA	1:F:952:ARG:HB2	1.92	0.51
1:B:185:LEU:HB2	1:B:756:ALA:HA	1.93	0.51
1:D:43:ALA:HB2	1:D:656:VAL:HG12	1.92	0.51
1:D:97:PHE:CZ	1:D:106:SER:HB3	2.46	0.51
1:F:9:CYS:HB2	1:F:481:LEU:HD23	1.92	0.51
1:F:376:LEU:HD12	1:F:470:PHE:HB3	1.91	0.51
1:C:403:VAL:HG21	1:C:436:ILE:HD11	1.92	0.51
1:C:836:TYR:HB3	1:C:837:ASP:HB2	1.90	0.51
1:D:87:THR:HB	1:D:798:THR:HG22	1.92	0.51
1:A:232:LEU:HD23	1:A:234:ARG:HH12	1.75	0.51
1:C:665:SER:OG	1:C:811:ARG:HB2	2.11	0.51
1:D:761:SER:HA	1:D:764:ASN:ND2	2.24	0.51
1:E:273:MET:HG3	1:E:274:ASP:H	1.74	0.51
1:B:858:ARG:O	1:B:862:ILE:HG13	2.10	0.51
1:C:376:LEU:HD12	1:C:470:PHE:HB3	1.93	0.51
1:D:698:ASP:OD2	1:D:815:ARG:NH1	2.32	0.51
1:E:597:ASN:HD22	1:E:599:GLU:H	1.56	0.51
1:F:665:SER:OG	1:F:811:ARG:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:697:GLN:HG2	1:F:815:ARG:CZ	2.41	0.51
1:B:557:LEU:HB3	1:B:611:THR:HB	1.93	0.51
1:C:575:ASP:OD1	1:C:578:ARG:NH2	2.42	0.51
1:F:87:THR:OG1	1:F:88:PHE:N	2.42	0.51
1:A:184:MET:HG3	1:A:263:GLY:HA3	1.92	0.51
1:A:761:SER:HA	1:A:764:ASN:HD22	1.76	0.51
1:C:140:TYR:CD1	1:C:317:VAL:HG23	2.46	0.51
1:C:448:LEU:HD22	1:C:451:PHE:HE2	1.76	0.51
1:A:920:LEU:HD21	1:A:996:GLY:HA3	1.92	0.51
1:B:273:MET:O	1:B:578:ARG:NE	2.42	0.51
1:B:281:GLN:OE1	1:B:320:TYR:OH	2.22	0.51
1:D:182:GLN:HG3	1:D:265:PRO:HD3	1.93	0.51
1:D:232:LEU:HD23	1:D:234:ARG:HH12	1.76	0.51
1:D:920:LEU:HD21	1:D:996:GLY:HA3	1.92	0.51
1:A:698:ASP:OD2	1:A:815:ARG:NH1	2.31	0.51
1:C:949:ALA:HA	1:C:952:ARG:HB2	1.92	0.51
1:E:185:LEU:HB2	1:E:756:ALA:HA	1.92	0.51
1:F:907:MET:HE1	1:F:988:PRO:HA	1.93	0.51
1:A:267:ARG:NH1	1:A:278:ASP:OD2	2.45	0.50
1:A:559:VAL:HG22	1:A:646:VAL:HG22	1.92	0.50
1:C:41:ASP:HA	1:C:134:ILE:HD11	1.94	0.50
1:F:575:ASP:OD1	1:F:578:ARG:NH2	2.40	0.50
1:C:697:GLN:HG2	1:C:815:ARG:CZ	2.41	0.50
1:D:761:SER:HA	1:D:764:ASN:HD22	1.75	0.50
1:D:969:ALA:HB1	1:D:994:VAL:HG13	1.93	0.50
1:F:448:LEU:HD22	1:F:451:PHE:HE2	1.76	0.50
1:A:653:ILE:HA	1:A:656:VAL:HG22	1.93	0.50
1:A:761:SER:HA	1:A:764:ASN:ND2	2.26	0.50
1:D:653:ILE:HA	1:D:656:VAL:HG22	1.93	0.50
1:D:669:VAL:HB	1:D:810:VAL:HB	1.93	0.50
1:F:671:VAL:HG22	1:F:843:VAL:HG22	1.93	0.50
1:F:817:ARG:HH11	1:F:822:PHE:HA	1.75	0.50
1:A:182:GLN:HG3	1:A:265:PRO:HD3	1.93	0.50
1:C:907:MET:HE1	1:C:988:PRO:HA	1.94	0.50
1:D:85:LYS:HE2	1:D:800:THR:HG22	1.94	0.50
1:A:87:THR:OG1	1:A:88:PHE:N	2.42	0.50
1:C:620:THR:O	1:C:620:THR:OG1	2.26	0.50
1:D:572:GLN:O	1:D:576:ASN:ND2	2.43	0.50
1:F:46:THR:HG21	1:F:659:LYS:HD2	1.94	0.50
1:F:468:VAL:O	1:F:472:LEU:HB2	2.12	0.50
1:F:689:LEU:O	1:F:692:THR:OG1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:653:ILE:O	1:E:657:LEU:HG	2.12	0.50
1:F:358:ALA:HA	1:F:361:ILE:HG12	1.93	0.50
1:A:669:VAL:HB	1:A:810:VAL:HB	1.94	0.50
1:B:53:VAL:HG21	1:B:65:ILE:HD13	1.94	0.50
1:E:749:ASP:HB2	1:F:71:ARG:HH22	1.77	0.50
1:F:41:ASP:HA	1:F:134:ILE:HD11	1.93	0.50
1:A:202:ILE:O	1:A:206:ILE:HG22	2.12	0.49
1:C:46:THR:HG21	1:C:659:LYS:HD2	1.94	0.49
1:F:403:VAL:HG21	1:F:436:ILE:HD11	1.93	0.49
1:B:749:ASP:HB2	1:C:71:ARG:HH22	1.75	0.49
1:D:202:ILE:O	1:D:206:ILE:HG22	2.12	0.49
1:D:387:LEU:HB3	1:D:985:VAL:HG11	1.94	0.49
1:F:189:PRO:HA	1:F:192:LEU:HD12	1.95	0.49
1:A:387:LEU:HB3	1:A:985:VAL:HG11	1.94	0.49
1:A:729:VAL:HG22	1:A:774:LEU:HD11	1.94	0.49
1:D:357:ARG:H	1:D:357:ARG:HD2	1.77	0.49
1:F:743:THR:OG1	1:F:744:GLN:N	2.45	0.49
1:F:969:ALA:HB2	1:F:997:LEU:HD23	1.94	0.49
1:C:82:MET:HG3	1:C:95:VAL:HG22	1.93	0.49
1:E:557:LEU:HB3	1:E:611:THR:HB	1.95	0.49
1:C:57:ALA:HA	1:C:88:PHE:HD1	1.77	0.49
1:D:35:PRO:HG2	1:D:383:PRO:HA	1.95	0.49
1:D:134:ILE:O	1:D:323:ARG:NH1	2.45	0.49
1:F:934:ASN:HD22	1:F:957:ARG:CZ	2.25	0.49
1:C:560:THR:HB	1:C:645:GLN:HB2	1.94	0.49
1:E:134:ILE:HB	1:E:652:MET:HE2	1.94	0.49
1:F:677:ALA:O	1:F:681:GLN:HG3	2.11	0.49
1:B:732:LEU:HD21	1:B:784:LEU:HD22	1.94	0.49
1:C:358:ALA:HA	1:C:361:ILE:HG12	1.93	0.49
1:E:732:LEU:HD21	1:E:784:LEU:HD22	1.95	0.49
1:B:67:ILE:HA	1:B:70:GLU:HG2	1.94	0.49
1:B:653:ILE:O	1:B:657:LEU:HG	2.12	0.49
1:D:15:ILE:HG12	1:E:875:PHE:CE2	2.48	0.49
1:F:510:TYR:CE2	1:F:955:GLY:HA2	2.48	0.49
1:B:176:PHE:CE1	1:B:593:GLN:HB3	2.47	0.49
1:B:393:ASP:OD1	1:B:396:ILE:N	2.44	0.49
1:C:577:LEU:HD13	1:C:644:THR:HG21	1.95	0.49
1:D:311:LEU:HD13	1:D:315:VAL:HG12	1.94	0.49
1:F:140:TYR:CD1	1:F:317:VAL:HG23	2.48	0.49
1:D:267:ARG:NH1	1:D:278:ASP:OD2	2.46	0.49
1:F:393:ASP:O	1:F:395:GLY:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLN:O	1:B:112:GLU:HG3	2.13	0.48
1:C:391:ALA:HB3	1:C:464:MET:HE2	1.95	0.48
1:C:969:ALA:HB2	1:C:997:LEU:HD23	1.94	0.48
1:D:729:VAL:HG22	1:D:774:LEU:HD11	1.95	0.48
1:B:306:LEU:HD23	1:B:310:ILE:HB	1.95	0.48
1:E:67:ILE:HA	1:E:70:GLU:HG2	1.95	0.48
1:E:104:TYR:O	1:E:108:GLN:HB2	2.13	0.48
1:E:676:PHE:HZ	1:E:799:ILE:HG23	1.78	0.48
1:F:560:THR:HB	1:F:645:GLN:HB2	1.94	0.48
1:F:726:VAL:O	1:F:730:MET:HG2	2.13	0.48
1:B:20:PHE:HA	1:B:23:VAL:HG12	1.96	0.48
1:B:449:PRO:HD3	1:B:866:VAL:HG11	1.94	0.48
1:C:934:ASN:HD22	1:C:957:ARG:CZ	2.25	0.48
1:F:577:LEU:HD13	1:F:644:THR:HG21	1.94	0.48
1:B:264:ASN:ND2	1:B:265:PRO:O	2.47	0.48
1:C:87:THR:OG1	1:C:88:PHE:N	2.47	0.48
1:C:402:ILE:HB	1:C:963:MET:HE3	1.95	0.48
1:E:108:GLN:O	1:E:112:GLU:HG3	2.13	0.48
1:E:189:PRO:HA	1:E:192:LEU:HD12	1.95	0.48
1:E:650:GLN:HB2	1:E:653:ILE:HG22	1.95	0.48
1:A:85:LYS:HE2	1:A:800:THR:HG22	1.95	0.48
1:A:134:ILE:O	1:A:323:ARG:NH1	2.45	0.48
1:A:140:TYR:HA	1:A:319:PRO:HA	1.95	0.48
1:B:521:THR:HB	1:B:1014:LEU:HD22	1.96	0.48
1:B:791:ARG:HH21	1:B:793:ALA:HB2	1.79	0.48
1:C:189:PRO:HA	1:C:192:LEU:HD12	1.94	0.48
1:C:438:PHE:HA	1:C:441:ILE:HG22	1.96	0.48
1:C:510:TYR:CE2	1:C:955:GLY:HA2	2.49	0.48
1:D:73:ILE:O	1:D:75:GLY:N	2.46	0.48
1:A:279:THR:OG1	1:A:280:ILE:N	2.39	0.48
1:A:441:ILE:HA	1:A:444:ILE:HG22	1.95	0.48
1:B:650:GLN:HB2	1:B:653:ILE:HG22	1.95	0.48
1:C:586:GLU:OE2	1:C:623:SER:OG	2.26	0.48
1:E:440:MET:HE3	1:E:441:ILE:HD12	1.96	0.48
1:A:73:ILE:O	1:A:75:GLY:N	2.46	0.48
1:B:104:TYR:O	1:B:108:GLN:HB2	2.14	0.48
1:B:134:ILE:HB	1:B:652:MET:HE2	1.96	0.48
1:C:468:VAL:O	1:C:472:LEU:HB2	2.13	0.48
1:C:677:ALA:O	1:C:681:GLN:HG3	2.13	0.48
1:F:791:ARG:HH21	1:F:793:ALA:HA	1.78	0.48
1:A:35:PRO:HG2	1:A:383:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ILE:HA	1:D:801:ARG:HH12	1.79	0.48
1:D:140:TYR:HA	1:D:319:PRO:HA	1.95	0.48
1:E:784:LEU:HG	1:E:790:ILE:HD11	1.96	0.48
1:A:406:GLU:HG2	1:A:960:PRO:HB3	1.95	0.48
1:B:61:VAL:HG11	1:B:90:LEU:O	2.14	0.48
1:B:189:PRO:HA	1:B:192:LEU:HD12	1.94	0.48
1:C:8:LEU:O	1:C:12:ARG:HB2	2.14	0.48
1:C:726:VAL:O	1:C:730:MET:HG2	2.13	0.48
1:D:441:ILE:HA	1:D:444:ILE:HG22	1.95	0.48
1:E:20:PHE:HA	1:E:23:VAL:HG12	1.95	0.48
1:F:57:ALA:HA	1:F:88:PHE:HD1	1.79	0.48
1:A:357:ARG:H	1:A:357:ARG:HD2	1.78	0.48
1:E:176:PHE:CE1	1:E:593:GLN:HB3	2.49	0.48
1:F:552:GLU:OE2	1:F:652:MET:HB2	2.14	0.48
1:C:791:ARG:HH21	1:C:793:ALA:HA	1.78	0.47
1:E:172:ASP:OD1	1:E:173:VAL:N	2.41	0.47
1:E:306:LEU:HD23	1:E:310:ILE:HB	1.95	0.47
1:F:402:ILE:HB	1:F:963:MET:HE3	1.96	0.47
1:F:894:ALA:HA	1:F:1000:ALA:HB2	1.96	0.47
1:A:311:LEU:HD13	1:A:315:VAL:HG12	1.96	0.47
1:A:698:ASP:O	1:A:812:LEU:HA	2.14	0.47
1:B:80:HIS:HB3	1:B:96:VAL:HG23	1.96	0.47
1:C:732:LEU:HD11	1:C:772:LEU:HD13	1.96	0.47
1:F:391:ALA:HB3	1:F:464:MET:HE2	1.97	0.47
1:B:73:ILE:HG22	1:B:82:MET:HE3	1.95	0.47
1:B:676:PHE:HZ	1:B:799:ILE:HG23	1.79	0.47
1:E:791:ARG:HH21	1:E:793:ALA:HB2	1.79	0.47
1:A:183:PHE:HB2	1:A:754:VAL:HA	1.96	0.47
1:A:241:ASN:OD1	1:A:241:ASN:N	2.46	0.47
1:B:73:ILE:HD11	1:B:114:ILE:HA	1.96	0.47
1:B:653:ILE:HA	1:B:656:VAL:HG22	1.96	0.47
1:E:42:ILE:O	1:E:459:LYS:NZ	2.45	0.47
1:E:53:VAL:HG21	1:E:65:ILE:HD13	1.95	0.47
1:F:732:LEU:HD11	1:F:772:LEU:HD13	1.97	0.47
1:B:440:MET:HE3	1:B:441:ILE:HD12	1.97	0.47
1:B:784:LEU:HG	1:B:790:ILE:HD11	1.97	0.47
1:D:690:LEU:HD22	1:D:812:LEU:HD13	1.97	0.47
1:E:521:THR:HB	1:E:1014:LEU:HD22	1.95	0.47
1:B:87:THR:OG1	1:B:88:PHE:N	2.47	0.47
1:C:671:VAL:HG22	1:C:843:VAL:HG22	1.95	0.47
1:D:691:LYS:HG3	1:D:699:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:ASP:O	1:D:812:LEU:HA	2.14	0.47
1:E:61:VAL:HG11	1:E:90:LEU:O	2.14	0.47
1:B:209:ASN:HB2	1:C:726:VAL:HG22	1.97	0.47
1:B:661:ALA:HB2	1:B:847:GLY:HA2	1.97	0.47
1:C:186:GLU:OE1	1:C:259:ARG:NH2	2.48	0.47
1:D:183:PHE:HB2	1:D:754:VAL:HA	1.96	0.47
1:D:203:THR:O	1:D:207:SER:OG	2.21	0.47
1:E:264:ASN:ND2	1:E:265:PRO:O	2.47	0.47
1:F:134:ILE:HB	1:F:652:MET:HE2	1.95	0.47
1:F:438:PHE:HA	1:F:441:ILE:HG22	1.96	0.47
1:F:586:GLU:OE2	1:F:625:ARG:NH1	2.48	0.47
1:F:959:ARG:HD3	1:F:959:ARG:HA	1.74	0.47
1:A:42:ILE:HG23	1:A:456:ILE:HB	1.96	0.47
1:B:385:ASN:HB3	1:B:463:PRO:HG2	1.97	0.47
1:B:569:LYS:HA	1:B:572:GLN:HE21	1.80	0.47
1:F:697:GLN:HG2	1:F:815:ARG:NH2	2.30	0.47
1:A:67:ILE:HA	1:A:801:ARG:HH12	1.80	0.47
1:A:440:MET:HG3	1:A:476:LEU:HD22	1.96	0.47
1:B:172:ASP:OD1	1:B:173:VAL:N	2.43	0.47
1:E:281:GLN:OE1	1:E:320:TYR:OH	2.23	0.47
1:E:385:ASN:HB3	1:E:463:PRO:HG2	1.97	0.47
1:F:578:ARG:O	1:F:582:MET:HG3	2.15	0.47
1:F:586:GLU:OE2	1:F:623:SER:OG	2.25	0.47
1:F:978:ALA:O	1:F:980:GLY:N	2.48	0.47
1:B:893:LEU:HD22	1:B:1003:LEU:HD13	1.97	0.47
1:C:393:ASP:O	1:C:395:GLY:N	2.43	0.47
1:D:166:GLN:HA	1:E:74:MET:HE3	1.97	0.47
1:E:73:ILE:HG22	1:E:82:MET:HE3	1.97	0.47
1:F:674:ASN:HA	1:F:806:ARG:HG3	1.97	0.47
1:A:690:LEU:HD22	1:A:812:LEU:HD13	1.97	0.46
1:C:697:GLN:HG2	1:C:815:ARG:NH2	2.30	0.46
1:C:894:ALA:HA	1:C:1000:ALA:HB2	1.97	0.46
1:D:51:THR:HG21	1:D:65:ILE:HG21	1.97	0.46
1:D:617:PRO:HB2	1:D:620:THR:OG1	2.14	0.46
1:E:31:TRP:HB2	1:E:374:PHE:CD1	2.50	0.46
1:E:893:LEU:HD22	1:E:1003:LEU:HD13	1.97	0.46
1:F:620:THR:O	1:F:620:THR:OG1	2.27	0.46
1:F:669:VAL:HG21	1:F:690:LEU:HD11	1.97	0.46
1:C:212:ASN:OD1	1:C:231:GLY:N	2.41	0.46
1:C:959:ARG:HA	1:C:959:ARG:HD3	1.74	0.46
1:D:268:HIS:HB3	1:D:596:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ASN:OD1	1:D:241:ASN:N	2.48	0.46
1:E:73:ILE:HD11	1:E:114:ILE:HA	1.97	0.46
1:A:111:GLN:NE2	1:A:114:ILE:HD11	2.31	0.46
1:D:1001:THR:HA	1:D:1004:THR:HG22	1.98	0.46
1:E:661:ALA:HB2	1:E:847:GLY:HA2	1.98	0.46
1:A:1001:THR:HA	1:A:1004:THR:HG22	1.98	0.46
1:B:31:TRP:HB2	1:B:374:PHE:CD1	2.51	0.46
1:B:588:GLU:HB3	1:B:616:HIS:CE1	2.50	0.46
1:C:584:PHE:HB3	1:C:586:GLU:OE1	2.16	0.46
1:C:978:ALA:O	1:C:980:GLY:N	2.48	0.46
1:E:144:SER:HB2	1:E:315:VAL:HG22	1.98	0.46
1:C:42:ILE:O	1:C:456:ILE:HG22	2.16	0.46
1:C:441:ILE:HG23	1:C:873:LEU:HD13	1.98	0.46
1:C:448:LEU:O	1:C:450:LEU:N	2.44	0.46
1:D:111:GLN:NE2	1:D:114:ILE:HD11	2.30	0.46
1:B:126:SER:OG	1:B:127:LEU:N	2.46	0.46
1:B:442:VAL:HA	1:B:445:THR:HG22	1.97	0.46
1:B:673:GLY:O	1:B:806:ARG:HB3	2.16	0.46
1:C:552:GLU:OE2	1:C:652:MET:HB2	2.14	0.46
1:C:673:GLY:O	1:C:806:ARG:HB2	2.16	0.46
1:A:51:THR:HG21	1:A:65:ILE:HG21	1.98	0.46
1:A:212:ASN:ND2	1:A:232:LEU:HD22	2.31	0.46
1:A:617:PRO:HB2	1:A:620:THR:OG1	2.15	0.46
1:C:134:ILE:HB	1:C:652:MET:HE2	1.97	0.46
1:C:669:VAL:HG21	1:C:690:LEU:HD11	1.98	0.46
1:D:42:ILE:HG23	1:D:456:ILE:HB	1.98	0.46
1:F:186:GLU:OE1	1:F:259:ARG:NH2	2.48	0.46
1:F:436:ILE:HD13	1:F:436:ILE:HA	1.75	0.46
1:B:929:ILE:HA	1:B:932:ILE:HG22	1.97	0.46
1:D:440:MET:HG3	1:D:476:LEU:HD22	1.97	0.46
1:F:632:GLU:OE1	1:F:815:ARG:NH2	2.48	0.46
1:A:669:VAL:HG21	1:A:690:LEU:HD11	1.98	0.45
1:B:217:ILE:HB	1:C:266:GLN:NE2	2.31	0.45
1:C:559:VAL:HG21	1:C:577:LEU:HD21	1.98	0.45
1:D:669:VAL:HG21	1:D:690:LEU:HD11	1.98	0.45
1:E:209:ASN:HB2	1:F:726:VAL:HG22	1.97	0.45
1:E:732:LEU:HD11	1:E:772:LEU:HD13	1.98	0.45
1:F:829:ARG:HA	1:F:832:LYS:HE3	1.98	0.45
1:A:137:ILE:HD13	1:A:286:LEU:HB2	1.99	0.45
1:A:910:ASN:OD1	1:A:912:SER:HB3	2.16	0.45
1:C:35:PRO:HG2	1:C:383:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:733:ILE:HD13	1:F:229:GLY:HA3	1.99	0.45
1:F:673:GLY:O	1:F:806:ARG:HB2	2.15	0.45
1:F:874:LEU:HD11	1:F:929:ILE:HD11	1.98	0.45
1:F:934:ASN:O	1:F:938:TRP:HB2	2.16	0.45
1:B:436:ILE:HD13	1:B:436:ILE:HA	1.84	0.45
1:B:883:GLN:HA	1:B:886:LEU:HG	1.98	0.45
1:D:406:GLU:HG2	1:D:960:PRO:HB3	1.96	0.45
1:E:625:ARG:HG3	1:E:629:GLN:HB2	1.99	0.45
1:B:969:ALA:HB2	1:B:997:LEU:HD13	1.98	0.45
1:C:16:VAL:HA	1:C:19:VAL:HG12	1.99	0.45
1:C:107:ARG:NH2	1:C:128:ASP:O	2.47	0.45
1:E:87:THR:OG1	1:E:88:PHE:N	2.49	0.45
1:F:155:LEU:HD13	1:F:315:VAL:HG11	1.99	0.45
1:B:746:PHE:CD1	1:C:64:GLN:HG2	2.52	0.45
1:E:80:HIS:HB3	1:E:96:VAL:HG23	1.97	0.45
1:B:450:LEU:HD11	1:B:915:VAL:HG13	1.99	0.45
1:B:970:LEU:HG	1:B:973:ILE:HD12	1.99	0.45
1:E:588:GLU:HB3	1:E:616:HIS:CE1	2.51	0.45
1:E:673:GLY:O	1:E:806:ARG:HB3	2.16	0.45
1:F:674:ASN:OD1	1:F:806:ARG:NH1	2.50	0.45
1:A:985:VAL:O	1:A:988:PRO:HD2	2.17	0.45
1:C:586:GLU:OE2	1:C:625:ARG:NH1	2.50	0.45
1:D:710:VAL:HG13	1:F:227:VAL:HG22	1.99	0.45
1:D:953:GLY:O	1:D:957:ARG:N	2.44	0.45
1:E:929:ILE:HA	1:E:932:ILE:HG22	1.98	0.45
1:F:8:LEU:O	1:F:12:ARG:HB2	2.16	0.45
1:F:542:ILE:HD13	1:F:903:HIS:CE1	2.52	0.45
1:A:268:HIS:HB3	1:A:596:ARG:O	2.16	0.45
1:A:691:LYS:HG3	1:A:699:VAL:HB	1.98	0.45
1:B:911:VAL:O	1:B:915:VAL:HG23	2.17	0.45
1:F:584:PHE:HB3	1:F:586:GLU:OE1	2.16	0.45
1:A:203:THR:O	1:A:207:SER:OG	2.22	0.45
1:A:872:VAL:HG13	1:C:18:LEU:HD23	1.99	0.45
1:C:155:LEU:HD13	1:C:315:VAL:HG11	1.98	0.45
1:C:542:ILE:HD13	1:C:903:HIS:CE1	2.52	0.45
1:C:791:ARG:NH2	1:C:792:LEU:O	2.50	0.45
1:D:109:ARG:O	1:D:112:GLU:HB2	2.17	0.45
1:D:436:ILE:HD13	1:D:436:ILE:HA	1.85	0.45
1:D:543:GLY:HA3	1:D:908:THR:HG22	1.99	0.45
1:D:910:ASN:OD1	1:D:912:SER:HB3	2.17	0.45
1:F:212:ASN:OD1	1:F:231:GLY:N	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:ASP:OD1	1:F:424:ASP:N	2.50	0.45
1:B:732:LEU:HD11	1:B:772:LEU:HD13	1.99	0.45
1:B:889:MET:O	1:B:892:PRO:HD2	2.17	0.45
1:C:320:TYR:CD1	1:C:321:ILE:HG13	2.52	0.45
1:C:829:ARG:HA	1:C:832:LYS:HE3	1.98	0.44
1:D:212:ASN:ND2	1:D:232:LEU:HD22	2.31	0.44
1:E:568:GLU:O	1:E:572:GLN:HG3	2.18	0.44
1:E:886:LEU:HD11	1:E:1015:ILE:HG21	1.99	0.44
1:F:320:TYR:CD1	1:F:321:ILE:HG13	2.51	0.44
1:A:33:GLN:HE21	1:A:33:GLN:HB2	1.61	0.44
1:B:144:SER:HB2	1:B:315:VAL:HG22	1.98	0.44
1:C:934:ASN:O	1:C:938:TRP:HB2	2.16	0.44
1:F:35:PRO:HG2	1:F:383:PRO:HA	1.99	0.44
1:F:400:GLY:HA3	1:F:440:MET:HE2	1.99	0.44
1:A:918:ILE:HD13	1:A:918:ILE:HA	1.81	0.44
1:C:632:GLU:OE1	1:C:815:ARG:NH2	2.49	0.44
1:C:674:ASN:HA	1:C:806:ARG:HG3	1.99	0.44
1:C:874:LEU:HD11	1:C:929:ILE:HD11	1.98	0.44
1:D:673:GLY:HA2	1:D:840:HIS:HB2	1.99	0.44
1:D:894:ALA:HA	1:D:1000:ALA:HB2	1.99	0.44
1:E:970:LEU:HG	1:E:973:ILE:HD12	1.99	0.44
1:F:791:ARG:NH2	1:F:792:LEU:O	2.50	0.44
1:A:139:ARG:HB2	1:A:321:ILE:HB	2.00	0.44
1:B:212:ASN:CG	1:B:232:LEU:HD13	2.43	0.44
1:E:746:PHE:CD1	1:F:64:GLN:HG2	2.52	0.44
1:F:441:ILE:HG23	1:F:873:LEU:HD13	1.97	0.44
1:A:56:LEU:HD21	1:C:212:ASN:O	2.18	0.44
1:E:653:ILE:HA	1:E:656:VAL:HG22	2.00	0.44
1:F:654:ASP:OD2	1:F:664:HIS:ND1	2.50	0.44
1:A:543:GLY:HA3	1:A:908:THR:HG22	2.00	0.44
1:C:424:ASP:OD1	1:C:424:ASP:N	2.50	0.44
1:C:514:LEU:HB3	1:C:951:VAL:HG22	1.99	0.44
1:C:588:GLU:HG2	1:C:589:HIS:CD2	2.53	0.44
1:D:236:LEU:HD23	1:D:236:LEU:H	1.82	0.44
1:F:408:ILE:O	1:F:412:ARG:HB3	2.17	0.44
1:F:897:GLY:HA3	1:F:996:GLY:HA2	2.00	0.44
1:A:73:ILE:HD11	1:A:114:ILE:HG22	2.00	0.44
1:B:1006:VAL:HG12	1:B:1007:LEU:HD23	2.00	0.44
1:D:742:VAL:N	1:D:754:VAL:O	2.51	0.44
1:E:442:VAL:HA	1:E:445:THR:HG22	1.98	0.44
1:E:969:ALA:HB2	1:E:997:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:GLU:O	1:A:829:ARG:HG3	2.18	0.44
1:B:9:CYS:SG	1:B:10:PHE:N	2.91	0.44
1:C:81:VAL:HB	1:C:96:VAL:HG13	2.00	0.44
1:C:408:ILE:O	1:C:412:ARG:HB3	2.18	0.44
1:C:578:ARG:O	1:C:582:MET:HG3	2.18	0.44
1:D:825:GLU:O	1:D:829:ARG:HG3	2.17	0.44
1:E:9:CYS:SG	1:E:10:PHE:N	2.91	0.44
1:F:42:ILE:O	1:F:456:ILE:HG22	2.18	0.44
1:F:905:ARG:NH1	1:F:976:ALA:O	2.43	0.44
1:B:448:LEU:HD21	1:B:865:MET:HE2	1.99	0.44
1:B:957:ARG:HH11	1:B:960:PRO:HG3	1.83	0.44
1:D:137:ILE:HD13	1:D:286:LEU:HB2	2.00	0.44
1:D:562:PRO:HD3	1:D:643:GLY:O	2.18	0.44
1:D:743:THR:OG1	1:D:744:GLN:N	2.51	0.44
1:D:918:ILE:HD13	1:D:918:ILE:HA	1.80	0.44
1:E:217:ILE:HB	1:F:266:GLN:NE2	2.33	0.44
1:E:368:LEU:O	1:E:372:MET:HG3	2.16	0.44
1:E:569:LYS:HA	1:E:572:GLN:HE21	1.82	0.44
1:E:883:GLN:HA	1:E:886:LEU:HG	1.99	0.44
1:E:957:ARG:HH11	1:E:960:PRO:HG3	1.83	0.44
1:F:355:SER:HA	1:F:356:PRO:HD2	1.90	0.44
1:A:726:VAL:HB	1:C:209:ASN:HB2	2.00	0.43
1:A:894:ALA:HA	1:A:1000:ALA:HB2	1.99	0.43
1:B:166:GLN:HE21	1:B:166:GLN:HB3	1.65	0.43
1:B:584:PHE:HA	1:B:585:PRO:HD3	1.83	0.43
1:D:56:LEU:HD21	1:F:212:ASN:O	2.17	0.43
1:D:411:ARG:HD2	1:D:411:ARG:HA	1.86	0.43
1:F:613:VAL:HG11	1:F:634:MET:HE1	1.99	0.43
1:C:400:GLY:HA3	1:C:440:MET:HE2	1.98	0.43
1:D:279:THR:OG1	1:D:280:ILE:N	2.36	0.43
1:E:932:ILE:HA	1:E:935:LEU:HB2	2.00	0.43
1:F:16:VAL:HA	1:F:19:VAL:HG12	1.99	0.43
1:A:673:GLY:HA2	1:A:840:HIS:HB2	2.00	0.43
1:B:450:LEU:HA	1:B:453:PHE:CE2	2.53	0.43
1:B:970:LEU:HA	1:B:973:ILE:HG13	2.00	0.43
1:C:436:ILE:HA	1:C:436:ILE:HD13	1.74	0.43
1:E:270:ILE:HB	1:E:594:VAL:HG13	2.00	0.43
1:E:295:VAL:O	1:E:299:VAL:HG23	2.19	0.43
1:E:977:LEU:HB3	1:E:979:HIS:NE2	2.33	0.43
1:F:562:PRO:HG2	1:F:565:ILE:HG13	1.99	0.43
1:A:366:ILE:HB	1:A:367:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:MET:C	1:C:584:PHE:H	2.25	0.43
1:C:654:ASP:OD2	1:C:664:HIS:ND1	2.52	0.43
1:D:366:ILE:HB	1:D:367:PRO:HD3	2.01	0.43
1:D:985:VAL:O	1:D:988:PRO:HD2	2.17	0.43
1:E:345:VAL:HG11	1:E:398:VAL:HG21	2.00	0.43
1:E:393:ASP:OD1	1:E:396:ILE:N	2.44	0.43
1:E:395:GLY:HA3	1:E:968:ALA:HA	2.00	0.43
1:E:1006:VAL:HG12	1:E:1007:LEU:HD23	2.00	0.43
1:F:210:ASN:OD1	1:F:233:ILE:HG22	2.18	0.43
1:A:361:ILE:HG23	1:A:486:LEU:HD12	2.01	0.43
1:B:977:LEU:HB3	1:B:979:HIS:NE2	2.33	0.43
1:C:206:ILE:CG2	1:C:742:VAL:HG11	2.49	0.43
1:D:361:ILE:HG23	1:D:486:LEU:HD12	2.00	0.43
1:E:911:VAL:O	1:E:915:VAL:HG23	2.18	0.43
1:F:582:MET:C	1:F:584:PHE:H	2.26	0.43
1:A:874:LEU:HB2	1:A:884:PRO:HB3	2.00	0.43
1:B:296:MET:HE2	1:B:300:HIS:CE1	2.53	0.43
1:C:562:PRO:HG2	1:C:565:ILE:HG13	2.00	0.43
1:D:165:LYS:HE2	1:D:165:LYS:HB3	1.81	0.43
1:E:450:LEU:HD11	1:E:915:VAL:HG13	2.00	0.43
1:F:588:GLU:HG2	1:F:589:HIS:CD2	2.54	0.43
1:F:823:LEU:O	1:F:827:ARG:HB3	2.19	0.43
1:A:897:GLY:HA3	1:A:996:GLY:HA2	2.01	0.43
1:B:368:LEU:O	1:B:372:MET:HG3	2.18	0.43
1:B:395:GLY:HA3	1:B:968:ALA:HA	2.01	0.43
1:C:210:ASN:OD1	1:C:233:ILE:HG22	2.19	0.43
1:D:368:LEU:O	1:D:372:MET:HG3	2.19	0.43
1:E:166:GLN:HE21	1:E:166:GLN:HB3	1.65	0.43
1:E:448:LEU:HD21	1:E:865:MET:HE2	2.00	0.43
1:F:88:PHE:HD2	1:F:596:ARG:HH22	1.67	0.43
1:B:625:ARG:HG3	1:B:629:GLN:HB2	1.99	0.43
1:B:973:ILE:N	1:B:974:PRO:HD2	2.33	0.43
1:C:268:HIS:HB2	1:C:269:GLY:H	1.70	0.43
1:C:897:GLY:HA3	1:C:996:GLY:HA2	2.01	0.43
1:E:212:ASN:CG	1:E:232:LEU:HD13	2.43	0.43
1:F:791:ARG:HE	1:F:793:ALA:HB2	1.83	0.43
1:A:236:LEU:H	1:A:236:LEU:HD23	1.83	0.43
1:A:368:LEU:O	1:A:372:MET:HG3	2.19	0.43
1:A:716:ARG:CZ	1:A:726:VAL:HG21	2.49	0.43
1:B:693:VAL:HA	1:B:694:PRO:HD3	1.94	0.43
1:C:287:LEU:HD23	1:C:290:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:970:LEU:HA	1:E:973:ILE:HG13	2.00	0.43
1:F:80:HIS:ND1	1:F:81:VAL:HG23	2.34	0.43
1:F:449:PRO:HB2	1:F:862:ILE:HG23	2.01	0.43
1:F:597:ASN:HB2	1:F:598:ASP:H	1.56	0.43
1:F:654:ASP:OD1	1:F:664:HIS:HB3	2.19	0.43
1:A:186:GLU:HB3	1:A:759:ILE:HG13	2.00	0.43
1:B:932:ILE:HA	1:B:935:LEU:HB2	2.00	0.43
1:C:674:ASN:OD1	1:C:806:ARG:NH1	2.52	0.43
1:E:54:ASN:HD21	1:E:268:HIS:CE1	2.37	0.43
1:E:133:PRO:HG2	1:E:656:VAL:HG12	2.01	0.43
1:E:296:MET:HE2	1:E:300:HIS:CE1	2.53	0.43
1:F:561:LEU:HB2	1:F:607:SER:O	2.19	0.43
1:A:411:ARG:HA	1:A:411:ARG:HD2	1.87	0.42
1:A:529:VAL:O	1:A:533:VAL:HG23	2.19	0.42
1:C:689:LEU:HD12	1:C:830:ILE:HD13	2.01	0.42
1:F:174:ALA:HB3	1:F:283:ILE:HB	2.01	0.42
1:F:833:GLU:HB2	1:F:834:VAL:H	1.49	0.42
1:F:950:VAL:O	1:F:954:ALA:HB3	2.19	0.42
1:C:704:GLU:OE2	1:C:704:GLU:N	2.51	0.42
1:D:561:LEU:HB2	1:D:607:SER:O	2.19	0.42
1:E:139:ARG:HB3	1:E:320:TYR:CZ	2.53	0.42
1:E:742:VAL:N	1:E:754:VAL:O	2.43	0.42
1:E:852:GLN:NE2	1:E:856:GLN:HE21	2.18	0.42
1:E:889:MET:O	1:E:892:PRO:HD2	2.18	0.42
1:F:81:VAL:HB	1:F:96:VAL:HG13	2.00	0.42
1:F:206:ILE:CG2	1:F:742:VAL:HG11	2.49	0.42
1:F:448:LEU:O	1:F:450:LEU:N	2.45	0.42
1:B:886:LEU:HD11	1:B:1015:ILE:HG21	2.00	0.42
1:C:174:ALA:HB3	1:C:283:ILE:HB	2.01	0.42
1:C:613:VAL:HG11	1:C:634:MET:HE1	2.00	0.42
1:C:722:LEU:HD12	1:C:787:VAL:HG13	2.01	0.42
1:C:823:LEU:O	1:C:827:ARG:HB3	2.19	0.42
1:D:911:VAL:O	1:D:915:VAL:HG23	2.20	0.42
1:E:391:ALA:HB3	1:E:464:MET:HE2	2.02	0.42
1:E:669:VAL:HG21	1:E:690:LEU:HD11	2.02	0.42
1:F:559:VAL:HG21	1:F:577:LEU:HD21	2.00	0.42
1:A:227:VAL:HG22	1:B:710:VAL:HG13	2.01	0.42
1:A:562:PRO:O	1:A:607:SER:OG	2.34	0.42
1:A:710:VAL:HG13	1:C:227:VAL:HG22	2.01	0.42
1:B:295:VAL:O	1:B:299:VAL:HG23	2.19	0.42
1:E:230:VAL:O	1:F:714:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.82	0.42
1:A:711:ARG:NH1	1:C:230:VAL:HG21	2.34	0.42
1:A:743:THR:OG1	1:A:744:GLN:N	2.53	0.42
1:A:972:LEU:HD12	1:A:993:VAL:HG11	2.02	0.42
1:B:42:ILE:O	1:B:459:LYS:NZ	2.47	0.42
1:B:75:GLY:O	1:B:113:ARG:NH2	2.52	0.42
1:C:444:ILE:HD11	1:C:472:LEU:HB3	2.02	0.42
1:C:449:PRO:HB2	1:C:862:ILE:HG23	2.02	0.42
1:C:517:LEU:HD22	1:C:1010:ALA:HB2	2.02	0.42
1:C:563:PRO:HB2	1:C:707:LEU:HD21	2.00	0.42
1:D:1003:LEU:HG	1:D:1007:LEU:HD13	2.02	0.42
1:E:741:PRO:HA	1:E:755:VAL:HG22	2.01	0.42
1:F:212:ASN:HD21	1:F:230:VAL:HG13	1.84	0.42
1:F:293:SER:O	1:F:297:GLU:HG3	2.18	0.42
1:B:345:VAL:HG11	1:B:398:VAL:HG21	2.01	0.42
1:C:504:VAL:O	1:C:508:PRO:HD3	2.20	0.42
1:C:654:ASP:OD1	1:C:664:HIS:HB3	2.20	0.42
1:D:213:ALA:HA	1:E:734:GLN:OE1	2.20	0.42
1:E:161:ILE:HG12	1:E:173:VAL:HG11	2.02	0.42
1:F:107:ARG:NH2	1:F:128:ASP:O	2.49	0.42
1:F:137:ILE:HD13	1:F:286:LEU:HD13	2.01	0.42
1:A:29:TYR:O	1:A:33:GLN:NE2	2.53	0.42
1:A:165:LYS:HB3	1:A:165:LYS:HE2	1.80	0.42
1:A:366:ILE:O	1:A:370:LEU:HG	2.20	0.42
1:A:730:MET:HE3	1:C:231:GLY:HA3	2.01	0.42
1:A:834:VAL:HA	1:A:835:PRO:HD3	1.77	0.42
1:B:139:ARG:HB3	1:B:320:TYR:CZ	2.54	0.42
1:B:568:GLU:O	1:B:572:GLN:HG3	2.18	0.42
1:B:749:ASP:HB2	1:C:71:ARG:NH2	2.34	0.42
1:B:961:VAL:HG11	1:B:1005:LEU:HD21	2.02	0.42
1:C:950:VAL:O	1:C:954:ALA:HB3	2.20	0.42
1:D:920:LEU:HD13	1:D:993:VAL:HA	2.00	0.42
1:E:973:ILE:N	1:E:974:PRO:HD2	2.33	0.42
1:F:287:LEU:HD23	1:F:290:GLU:HG3	2.01	0.42
1:A:12:ARG:O	1:A:16:VAL:HG22	2.20	0.42
1:C:293:SER:O	1:C:297:GLU:HG3	2.20	0.42
1:C:355:SER:HA	1:C:356:PRO:HD2	1.90	0.42
1:D:40:PRO:HG3	1:D:385:ASN:OD1	2.20	0.42
1:D:83:ARG:HG2	1:D:802:GLU:OE2	2.19	0.42
1:D:529:VAL:O	1:D:533:VAL:HG23	2.19	0.42
1:E:31:TRP:C	1:E:33:GLN:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:852:GLN:HE22	1:E:856:GLN:HE21	1.67	0.42
1:F:196:ASN:HD21	1:F:779:GLY:HA2	1.85	0.42
1:A:109:ARG:O	1:A:112:GLU:HB2	2.19	0.42
1:A:291:ASN:HA	1:A:292:PRO:HD3	1.89	0.42
1:A:344:LEU:HB3	1:A:970:LEU:HG	2.02	0.42
1:B:885:ALA:O	1:B:889:MET:HG2	2.20	0.42
1:C:858:ARG:HA	1:C:858:ARG:HD3	1.87	0.42
1:D:10:PHE:O	1:D:13:ARG:HG3	2.20	0.42
1:D:186:GLU:HB3	1:D:759:ILE:HG13	2.01	0.42
1:D:352:PHE:HD2	1:D:963:MET:HE2	1.85	0.42
1:E:206:ILE:HG12	1:E:742:VAL:HG11	2.02	0.42
1:E:353:LEU:HD12	1:E:353:LEU:HA	1.85	0.42
1:E:665:SER:OG	1:E:811:ARG:HB2	2.20	0.42
1:F:87:THR:HG21	1:F:603:PRO:HB2	2.02	0.42
1:F:279:THR:OG1	1:F:280:ILE:N	2.52	0.42
1:A:920:LEU:HD13	1:A:993:VAL:HA	2.01	0.42
1:B:54:ASN:HD21	1:B:268:HIS:CE1	2.37	0.42
1:B:197:ILE:HA	1:B:201:GLN:NE2	2.35	0.42
1:B:852:GLN:NE2	1:B:856:GLN:HE21	2.18	0.42
1:C:268:HIS:CD2	1:C:268:HIS:H	2.37	0.42
1:C:279:THR:OG1	1:C:280:ILE:N	2.50	0.42
1:C:729:VAL:O	1:C:732:LEU:HB3	2.20	0.42
1:C:963:MET:O	1:C:967:VAL:HG22	2.20	0.42
1:D:56:LEU:HD23	1:D:56:LEU:HA	1.90	0.42
1:D:73:ILE:HD11	1:D:114:ILE:HG22	2.02	0.42
1:D:230:VAL:HG21	1:E:711:ARG:HE	1.84	0.42
1:D:658:ASP:HB2	1:D:664:HIS:CD2	2.54	0.42
1:D:972:LEU:HD12	1:D:993:VAL:HG11	2.02	0.42
1:E:745:VAL:HG13	1:E:752:TYR:HB2	2.02	0.42
1:E:978:ALA:HA	1:E:987:ARG:HD3	2.02	0.42
1:F:39:TYR:HB3	1:F:652:MET:HE1	2.02	0.42
1:F:268:HIS:CD2	1:F:268:HIS:H	2.37	0.42
1:A:56:LEU:HD11	1:A:121:TYR:CE2	2.55	0.41
1:A:161:ILE:HG23	1:A:173:VAL:HB	2.02	0.41
1:A:456:ILE:HD11	1:A:546:PHE:CE1	2.55	0.41
1:A:658:ASP:HB2	1:A:664:HIS:CD2	2.54	0.41
1:C:87:THR:HG21	1:C:603:PRO:HB2	2.01	0.41
1:D:12:ARG:O	1:D:16:VAL:HG22	2.20	0.41
1:D:234:ARG:HB2	1:D:238:ASP:OD2	2.20	0.41
1:D:834:VAL:HA	1:D:835:PRO:HD3	1.77	0.41
1:E:75:GLY:O	1:E:113:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:TRP:O	1:E:109:ARG:HG2	2.19	0.41
1:E:450:LEU:HA	1:E:453:PHE:CE2	2.54	0.41
1:A:352:PHE:HD2	1:A:963:MET:HE2	1.85	0.41
1:B:270:ILE:HB	1:B:594:VAL:HG13	2.01	0.41
1:B:374:PHE:HD2	1:B:377:MET:HE2	1.85	0.41
1:B:669:VAL:HG21	1:B:690:LEU:HD11	2.01	0.41
1:D:34:LEU:HD12	1:D:34:LEU:HA	1.92	0.41
1:D:56:LEU:HD11	1:D:121:TYR:CE2	2.55	0.41
1:D:874:LEU:HB2	1:D:884:PRO:HB3	2.01	0.41
1:E:60:GLU:H	1:E:60:GLU:HG2	1.59	0.41
1:E:197:ILE:HA	1:E:201:GLN:NE2	2.36	0.41
1:F:126:SER:OG	1:F:127:LEU:N	2.52	0.41
1:F:514:LEU:HB3	1:F:951:VAL:HG22	2.00	0.41
1:F:517:LEU:HD22	1:F:1010:ALA:HB2	2.02	0.41
1:A:83:ARG:HG2	1:A:802:GLU:OE2	2.20	0.41
1:A:234:ARG:HB2	1:A:238:ASP:OD2	2.20	0.41
1:A:693:VAL:HA	1:A:694:PRO:HD3	1.88	0.41
1:B:358:ALA:O	1:B:361:ILE:HG22	2.20	0.41
1:B:978:ALA:HA	1:B:987:ARG:HD3	2.03	0.41
1:C:81:VAL:HA	1:C:803:MET:HE2	2.00	0.41
1:D:139:ARG:HB2	1:D:321:ILE:HB	2.02	0.41
1:F:565:ILE:HG22	1:F:566:SER:O	2.20	0.41
1:A:10:PHE:O	1:A:13:ARG:HG3	2.19	0.41
1:A:48:GLN:HG3	1:A:659:LYS:HZ1	1.85	0.41
1:B:830:ILE:O	1:B:834:VAL:HG22	2.20	0.41
1:C:88:PHE:HD2	1:C:596:ARG:HH22	1.69	0.41
1:C:344:LEU:O	1:C:348:VAL:HG23	2.20	0.41
1:C:791:ARG:HE	1:C:793:ALA:HB2	1.84	0.41
1:E:292:PRO:O	1:E:296:MET:HB2	2.20	0.41
1:E:358:ALA:HA	1:E:361:ILE:HG22	2.02	0.41
1:F:81:VAL:HA	1:F:803:MET:HE2	2.02	0.41
1:F:563:PRO:HB2	1:F:707:LEU:HD21	2.01	0.41
1:F:693:VAL:HA	1:F:694:PRO:HD3	1.89	0.41
1:F:836:TYR:HA	1:F:837:ASP:HA	1.92	0.41
1:A:266:GLN:NE2	1:C:217:ILE:HB	2.36	0.41
1:A:1006:VAL:HG12	1:A:1007:LEU:HD12	2.02	0.41
1:B:741:PRO:HA	1:B:755:VAL:HG22	2.01	0.41
1:B:745:VAL:HG13	1:B:752:TYR:HB2	2.02	0.41
1:B:920:LEU:HD21	1:B:996:GLY:HA3	2.02	0.41
1:C:31:TRP:HB2	1:C:374:PHE:CD1	2.56	0.41
1:D:32:LYS:HD3	1:D:32:LYS:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LEU:HB3	1:D:970:LEU:HG	2.03	0.41
1:D:897:GLY:HA3	1:D:996:GLY:HA2	2.02	0.41
1:F:276:ASN:HA	1:F:277:PRO:HD3	1.86	0.41
1:B:187:PHE:HE2	1:B:756:ALA:HB1	1.85	0.41
1:B:358:ALA:HA	1:B:361:ILE:HG22	2.02	0.41
1:C:938:TRP:HZ3	1:C:952:ARG:HH21	1.69	0.41
1:D:654:ASP:OD1	1:D:664:HIS:HB3	2.21	0.41
1:D:842:GLN:HE21	1:D:842:GLN:HB3	1.62	0.41
1:E:358:ALA:O	1:E:361:ILE:HG22	2.20	0.41
1:E:830:ILE:O	1:E:834:VAL:HG22	2.20	0.41
1:E:920:LEU:HD21	1:E:996:GLY:HA3	2.03	0.41
1:F:444:ILE:HD11	1:F:472:LEU:HB3	2.01	0.41
1:F:957:ARG:HD3	1:F:957:ARG:HA	1.73	0.41
1:F:963:MET:O	1:F:967:VAL:HG22	2.21	0.41
1:A:40:PRO:HG3	1:A:385:ASN:OD1	2.21	0.41
1:A:446:ALA:O	1:A:449:PRO:HD2	2.21	0.41
1:B:161:ILE:HG12	1:B:173:VAL:HG11	2.03	0.41
1:B:744:GLN:NE2	1:B:751:SER:OG	2.40	0.41
1:C:273:MET:O	1:C:578:ARG:NE	2.54	0.41
1:D:584:PHE:HB3	1:D:586:GLU:OE1	2.20	0.41
1:D:608:HIS:CE1	1:D:610:GLU:HG3	2.56	0.41
1:E:885:ALA:O	1:E:889:MET:HG2	2.21	0.41
1:E:961:VAL:HG11	1:E:1005:LEU:HD21	2.02	0.41
1:F:559:VAL:HB	1:F:609:ILE:HB	2.01	0.41
1:F:729:VAL:O	1:F:732:LEU:HB3	2.20	0.41
1:A:561:LEU:HB2	1:A:607:SER:O	2.21	0.41
1:B:391:ALA:HB3	1:B:464:MET:HE2	2.02	0.41
1:D:161:ILE:HG23	1:D:173:VAL:HB	2.02	0.41
1:D:674:ASN:CG	1:D:806:ARG:HH21	2.29	0.41
1:E:92:LEU:HD21	1:E:603:PRO:HB3	2.03	0.41
1:F:826:ALA:O	1:F:830:ILE:HG12	2.21	0.41
1:A:32:LYS:HA	1:A:32:LYS:HD3	1.89	0.41
1:A:39:TYR:HB3	1:A:652:MET:HE1	2.02	0.41
1:A:276:ASN:ND2	1:A:279:THR:HB	2.35	0.41
1:A:584:PHE:HB3	1:A:586:GLU:OE1	2.21	0.41
1:A:674:ASN:CG	1:A:806:ARG:HH21	2.29	0.41
1:A:1003:LEU:HG	1:A:1007:LEU:HD13	2.02	0.41
1:B:243:VAL:HB	1:C:725:ASN:OD1	2.20	0.41
1:C:80:HIS:ND1	1:C:81:VAL:HG23	2.36	0.41
1:C:138:TYR:CE2	1:C:319:PRO:HB3	2.56	0.41
1:C:514:LEU:HD13	1:C:951:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:617:PRO:HB2	1:C:620:THR:HG22	2.03	0.41
1:C:859:LEU:HD21	1:C:914:ALA:HB1	2.03	0.41
1:D:29:TYR:O	1:D:33:GLN:NE2	2.54	0.41
1:D:39:TYR:HB3	1:D:652:MET:HE1	2.03	0.41
1:D:83:ARG:NH1	1:D:660:LEU:O	2.49	0.41
1:D:291:ASN:HA	1:D:292:PRO:HD3	1.90	0.41
1:D:716:ARG:CZ	1:D:726:VAL:HG21	2.51	0.41
1:E:275:ARG:HG3	1:E:582:MET:HE1	2.03	0.41
1:E:468:VAL:O	1:E:472:LEU:HB2	2.21	0.41
1:E:556:TRP:HB2	1:E:651:PRO:N	2.36	0.41
1:F:31:TRP:HB2	1:F:374:PHE:CD1	2.56	0.41
1:F:235:ASN:ND2	1:F:237:ASP:OD2	2.54	0.41
1:F:344:LEU:O	1:F:348:VAL:HG23	2.20	0.41
1:F:689:LEU:HD12	1:F:830:ILE:HD13	2.02	0.41
1:A:911:VAL:O	1:A:915:VAL:HG23	2.21	0.41
1:B:206:ILE:HG12	1:B:742:VAL:HG11	2.02	0.41
1:B:783:ALA:O	1:B:786:GLN:HG2	2.20	0.41
1:D:366:ILE:O	1:D:370:LEU:HG	2.20	0.41
1:F:107:ARG:HD3	1:F:130:LEU:HD13	2.03	0.41
1:F:273:MET:O	1:F:578:ARG:NE	2.54	0.41
1:F:722:LEU:HD12	1:F:787:VAL:HG13	2.02	0.41
1:F:938:TRP:HZ3	1:F:952:ARG:HH21	1.69	0.41
1:A:21:ALA:O	1:A:25:LEU:HG	2.21	0.40
1:A:210:ASN:O	1:A:210:ASN:ND2	2.55	0.40
1:B:292:PRO:O	1:B:296:MET:HB2	2.21	0.40
1:C:561:LEU:HB2	1:C:607:SER:O	2.21	0.40
1:D:53:VAL:HG22	1:D:123:ALA:HB2	2.02	0.40
1:F:34:LEU:HD12	1:F:34:LEU:HA	1.96	0.40
1:F:791:ARG:NE	1:F:793:ALA:HB2	2.36	0.40
1:F:866:VAL:HG22	1:F:870:MET:HE3	2.03	0.40
1:A:736:GLY:O	1:A:758:PHE:HB2	2.22	0.40
1:A:893:LEU:HD22	1:A:1003:LEU:HD22	2.04	0.40
1:C:137:ILE:HD13	1:C:286:LEU:HD13	2.03	0.40
1:C:826:ALA:O	1:C:830:ILE:HG12	2.21	0.40
1:C:871:PHE:HB2	1:C:888:LEU:HD21	2.03	0.40
1:E:203:THR:HG21	1:E:735:THR:HG21	2.04	0.40
1:E:374:PHE:HD2	1:E:377:MET:HE2	1.85	0.40
1:E:436:ILE:HA	1:E:436:ILE:HD13	1.84	0.40
1:F:617:PRO:HB2	1:F:620:THR:HG22	2.03	0.40
1:F:859:LEU:HD21	1:F:914:ALA:HB1	2.03	0.40
1:A:157:PHE:CE2	1:A:180:THR:HG22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:HA	1:A:548:PRO:HD2	1.96	0.40
1:A:562:PRO:HD3	1:A:643:GLY:O	2.21	0.40
1:A:608:HIS:CE1	1:A:610:GLU:HG3	2.57	0.40
1:A:742:VAL:N	1:A:754:VAL:O	2.54	0.40
1:A:830:ILE:HD12	1:A:845:TRP:CZ2	2.57	0.40
1:B:133:PRO:HG2	1:B:656:VAL:HG12	2.03	0.40
1:B:203:THR:HG21	1:B:735:THR:HG21	2.02	0.40
1:C:295:VAL:O	1:C:299:VAL:HG23	2.21	0.40
1:C:913:SER:HB3	1:C:988:PRO:HB3	2.03	0.40
1:E:559:VAL:HG22	1:E:646:VAL:HG22	2.03	0.40
1:E:584:PHE:HA	1:E:585:PRO:HD3	1.82	0.40
1:E:690:LEU:HD21	1:E:830:ILE:HD11	2.02	0.40
1:F:138:TYR:CE2	1:F:319:PRO:HB3	2.56	0.40
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.92	0.40
1:B:36:LEU:HA	1:B:36:LEU:HD23	1.82	0.40
1:C:507:ALA:HA	1:C:958:MET:HE1	2.04	0.40
1:C:546:PHE:CD2	1:C:851:ASN:HB3	2.57	0.40
1:C:565:ILE:HG22	1:C:566:SER:O	2.21	0.40
1:D:276:ASN:ND2	1:D:279:THR:HB	2.36	0.40
1:D:446:ALA:O	1:D:449:PRO:HD2	2.22	0.40
1:D:544:ARG:HB2	1:D:820:SER:OG	2.21	0.40
1:E:187:PHE:HE2	1:E:756:ALA:HB1	1.86	0.40
1:E:894:ALA:HB1	1:E:920:LEU:HG	2.03	0.40
1:F:388:SER:HB2	1:F:464:MET:HE3	2.04	0.40
1:A:232:LEU:HD12	1:A:232:LEU:HA	1.93	0.40
1:A:400:GLY:O	1:A:403:VAL:HG22	2.21	0.40
1:A:544:ARG:HB2	1:A:820:SER:OG	2.21	0.40
1:A:703:GLN:HE21	1:A:800:THR:HG21	1.86	0.40
1:B:271:LEU:CD2	1:B:281:GLN:HB3	2.48	0.40
1:C:743:THR:OG1	1:C:744:GLN:N	2.46	0.40
1:D:456:ILE:HD11	1:D:546:PHE:CE1	2.56	0.40
1:D:703:GLN:HE21	1:D:800:THR:HG21	1.86	0.40
1:E:783:ALA:O	1:E:786:GLN:HG2	2.21	0.40
1:F:504:VAL:O	1:F:508:PRO:HD3	2.20	0.40
1:F:556:TRP:CZ2	1:F:610:GLU:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	944/1045 (90%)	837 (89%)	92 (10%)	15 (2%)	7	34
1	B	936/1045 (90%)	858 (92%)	76 (8%)	2 (0%)	43	76
1	C	943/1045 (90%)	850 (90%)	82 (9%)	11 (1%)	10	40
1	D	944/1045 (90%)	836 (89%)	93 (10%)	15 (2%)	7	34
1	E	936/1045 (90%)	860 (92%)	74 (8%)	2 (0%)	43	76
1	F	943/1045 (90%)	851 (90%)	81 (9%)	11 (1%)	10	40
All	All	5646/6270 (90%)	5092 (90%)	498 (9%)	56 (1%)	12	45

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	PHE
1	C	979	HIS
1	D	88	PHE
1	F	979	HIS
1	A	74	MET
1	A	120	PRO
1	C	268	HIS
1	C	274	ASP
1	D	74	MET
1	D	120	PRO
1	F	268	HIS
1	F	274	ASP
1	A	117	VAL
1	C	41	ASP
1	C	193	SER
1	D	117	VAL
1	F	41	ASP
1	F	193	SER
1	A	121	TYR
1	A	545	ASP

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Mol	Chain	Res	Type
1	A	626	ASP
1	A	818	ASP
1	A	978	ALA
1	A	979	HIS
1	B	651	PRO
1	C	985	VAL
1	D	121	TYR
1	D	545	ASP
1	D	626	ASP
1	D	818	ASP
1	D	978	ALA
1	D	979	HIS
1	E	651	PRO
1	F	985	VAL
1	A	209	ASN
1	A	780	ALA
1	B	623	SER
1	C	833	GLU
1	D	780	ALA
1	E	623	SER
1	F	481	LEU
1	F	833	GLU
1	C	481	LEU
1	D	77	PRO
1	D	209	ASN
1	A	77	PRO
1	A	651	PRO
1	D	651	PRO
1	F	462	SER
1	F	603	PRO
1	C	364	VAL
1	C	462	SER
1	F	364	VAL
1	A	953	GLY
1	D	953	GLY
1	C	603	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	787/864 (91%)	741 (94%)	46 (6%)	18	51
1	B	784/864 (91%)	745 (95%)	39 (5%)	22	56
1	C	789/864 (91%)	734 (93%)	55 (7%)	14	44
1	D	787/864 (91%)	744 (94%)	43 (6%)	19	53
1	E	784/864 (91%)	744 (95%)	40 (5%)	21	55
1	F	789/864 (91%)	734 (93%)	55 (7%)	14	44
All	All	4720/5184 (91%)	4442 (94%)	278 (6%)	18	50

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	49	VAL
1	A	56	LEU
1	A	93	ILE
1	A	96	VAL
1	A	126	SER
1	A	127	LEU
1	A	192	LEU
1	A	197	ILE
1	A	241	ASN
1	A	261	VAL
1	A	262	LEU
1	A	299	VAL
1	A	314	ASP
1	A	318	VAL
1	A	344	LEU
1	A	380	PHE
1	A	389	LEU
1	A	392	ILE
1	A	402	ILE
1	A	403	VAL
1	A	438	PHE
1	A	456	ILE
1	A	472	LEU
1	A	535	VAL
1	A	592	THR
1	A	594	VAL

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Mol	Chain	Res	Type
1	A	601	THR
1	A	626	ASP
1	A	689	LEU
1	A	692	THR
1	A	710	VAL
1	A	722	LEU
1	A	728	ASP
1	A	745	VAL
1	A	759	ILE
1	A	814	LEU
1	A	861	VAL
1	A	866	VAL
1	A	888	LEU
1	A	910	ASN
1	A	918	ILE
1	A	930	ILE
1	A	932	ILE
1	A	1005	LEU
1	A	1013	TYR
1	B	6	VAL
1	B	34	LEU
1	B	49	VAL
1	B	60	GLU
1	B	76	VAL
1	B	87	THR
1	B	96	VAL
1	B	108	GLN
1	B	131	THR
1	B	170	VAL
1	B	180	THR
1	B	206	ILE
1	B	233	ILE
1	B	260	VAL
1	B	276	ASN
1	B	317	VAL
1	B	375	ILE
1	B	440	MET
1	B	441	ILE
1	B	456	ILE
1	B	472	LEU
1	B	594	VAL
1	B	615	LEU

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Mol	Chain	Res	Type
1	B	620	THR
1	B	687	THR
1	B	700	ILE
1	B	710	VAL
1	B	726	VAL
1	B	728	ASP
1	B	814	LEU
1	B	818	ASP
1	B	849	PHE
1	B	856	GLN
1	B	873	LEU
1	B	875	PHE
1	B	910	ASN
1	B	986	GLN
1	B	989	LEU
1	B	997	LEU
1	C	9	CYS
1	C	33	GLN
1	C	34	LEU
1	C	49	VAL
1	C	56	LEU
1	C	60	GLU
1	C	64	GLN
1	C	96	VAL
1	C	173	VAL
1	C	218	LEU
1	C	236	LEU
1	C	237	ASP
1	C	260	VAL
1	C	262	LEU
1	C	271	LEU
1	C	274	ASP
1	C	317	VAL
1	C	318	VAL
1	C	347	LEU
1	C	429	VAL
1	C	436	ILE
1	C	444	ILE
1	C	447	TYR
1	C	472	LEU
1	C	481	LEU
1	C	504	VAL

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Mol	Chain	Res	Type
1	C	523	THR
1	C	550	LEU
1	C	561	LEU
1	C	594	VAL
1	C	597	ASN
1	C	619	SER
1	C	620	THR
1	C	632	GLU
1	C	636	THR
1	C	656	VAL
1	C	666	ASP
1	C	700	ILE
1	C	710	VAL
1	C	724	ILE
1	C	726	VAL
1	C	740	SER
1	C	792	LEU
1	C	798	THR
1	C	808	LEU
1	C	814	LEU
1	C	834	VAL
1	C	859	LEU
1	C	863	LEU
1	C	910	ASN
1	C	923	VAL
1	C	932	ILE
1	C	938	TRP
1	C	973	ILE
1	C	1013	TYR
1	D	33	GLN
1	D	49	VAL
1	D	56	LEU
1	D	93	ILE
1	D	96	VAL
1	D	126	SER
1	D	127	LEU
1	D	192	LEU
1	D	197	ILE
1	D	241	ASN
1	D	261	VAL
1	D	299	VAL
1	D	314	ASP

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Mol	Chain	Res	Type
1	D	344	LEU
1	D	380	PHE
1	D	389	LEU
1	D	392	ILE
1	D	402	ILE
1	D	403	VAL
1	D	438	PHE
1	D	456	ILE
1	D	472	LEU
1	D	535	VAL
1	D	592	THR
1	D	594	VAL
1	D	601	THR
1	D	626	ASP
1	D	689	LEU
1	D	692	THR
1	D	710	VAL
1	D	722	LEU
1	D	728	ASP
1	D	745	VAL
1	D	759	ILE
1	D	814	LEU
1	D	861	VAL
1	D	866	VAL
1	D	888	LEU
1	D	910	ASN
1	D	930	ILE
1	D	932	ILE
1	D	1005	LEU
1	D	1013	TYR
1	E	6	VAL
1	E	34	LEU
1	E	49	VAL
1	E	60	GLU
1	E	76	VAL
1	E	87	THR
1	E	96	VAL
1	E	108	GLN
1	E	131	THR
1	E	170	VAL
1	E	180	THR
1	E	206	ILE

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Mol	Chain	Res	Type
1	E	233	ILE
1	E	260	VAL
1	E	276	ASN
1	E	317	VAL
1	E	375	ILE
1	E	440	MET
1	E	441	ILE
1	E	456	ILE
1	E	472	LEU
1	E	594	VAL
1	E	615	LEU
1	E	620	THR
1	E	687	THR
1	E	700	ILE
1	E	710	VAL
1	E	726	VAL
1	E	728	ASP
1	E	806	ARG
1	E	814	LEU
1	E	818	ASP
1	E	849	PHE
1	E	856	GLN
1	E	873	LEU
1	E	875	PHE
1	E	910	ASN
1	E	986	GLN
1	E	989	LEU
1	E	997	LEU
1	F	9	CYS
1	F	33	GLN
1	F	34	LEU
1	F	49	VAL
1	F	56	LEU
1	F	60	GLU
1	F	64	GLN
1	F	91	SER
1	F	96	VAL
1	F	173	VAL
1	F	218	LEU
1	F	236	LEU
1	F	237	ASP
1	F	260	VAL

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Mol	Chain	Res	Type
1	F	262	LEU
1	F	271	LEU
1	F	274	ASP
1	F	317	VAL
1	F	318	VAL
1	F	347	LEU
1	F	429	VAL
1	F	436	ILE
1	F	444	ILE
1	F	447	TYR
1	F	472	LEU
1	F	481	LEU
1	F	504	VAL
1	F	523	THR
1	F	550	LEU
1	F	561	LEU
1	F	594	VAL
1	F	597	ASN
1	F	619	SER
1	F	620	THR
1	F	632	GLU
1	F	636	THR
1	F	656	VAL
1	F	666	ASP
1	F	700	ILE
1	F	710	VAL
1	F	724	ILE
1	F	726	VAL
1	F	740	SER
1	F	792	LEU
1	F	798	THR
1	F	808	LEU
1	F	814	LEU
1	F	834	VAL
1	F	859	LEU
1	F	863	LEU
1	F	910	ASN
1	F	932	ILE
1	F	938	TRP
1	F	973	ILE
1	F	1013	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	219	ASN
1	A	246	GLN
1	A	276	ASN
1	A	300	HIS
1	A	332	HIS
1	A	378	HIS
1	A	379	HIS
1	A	664	HIS
1	A	764	ASN
1	A	786	GLN
1	A	842	GLN
1	A	934	ASN
1	B	48	GLN
1	B	52	GLN
1	B	54	ASN
1	B	166	GLN
1	B	201	GLN
1	B	219	ASN
1	B	223	GLN
1	B	264	ASN
1	B	276	ASN
1	B	300	HIS
1	B	378	HIS
1	B	407	ASN
1	B	572	GLN
1	B	597	ASN
1	B	753	ASN
1	B	771	ASN
1	B	848	GLN
1	B	856	GLN
1	B	936	ASN
1	C	111	GLN
1	C	182	GLN
1	C	196	ASN
1	C	204	GLN
1	C	219	ASN
1	C	266	GLN
1	C	268	HIS
1	C	289	ASN
1	C	645	GLN
1	C	753	ASN

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Mol	Chain	Res	Type
1	C	764	ASN
1	C	807	HIS
1	C	848	GLN
1	C	851	ASN
1	C	934	ASN
1	D	33	GLN
1	D	124	GLN
1	D	219	ASN
1	D	246	GLN
1	D	276	ASN
1	D	300	HIS
1	D	378	HIS
1	D	379	HIS
1	D	664	HIS
1	D	764	ASN
1	D	786	GLN
1	D	842	GLN
1	D	853	GLN
1	D	934	ASN
1	E	48	GLN
1	E	52	GLN
1	E	54	ASN
1	E	64	GLN
1	E	166	GLN
1	E	201	GLN
1	E	276	ASN
1	E	300	HIS
1	E	407	ASN
1	E	572	GLN
1	E	597	ASN
1	E	753	ASN
1	E	771	ASN
1	E	848	GLN
1	E	856	GLN
1	E	936	ASN
1	F	111	GLN
1	F	182	GLN
1	F	196	ASN
1	F	204	GLN
1	F	219	ASN
1	F	266	GLN
1	F	268	HIS

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Mol	Chain	Res	Type
1	F	289	ASN
1	F	645	GLN
1	F	753	ASN
1	F	764	ASN
1	F	807	HIS
1	F	848	GLN
1	F	851	ASN
1	F	934	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	958/1045 (91%)	-0.72	1 (0%) 92 86	29, 77, 143, 215	0
1	B	954/1045 (91%)	-0.79	0 100 100	27, 70, 135, 209	0
1	C	959/1045 (91%)	-0.76	1 (0%) 92 86	26, 71, 140, 241	0
1	D	958/1045 (91%)	-0.72	1 (0%) 92 86	29, 77, 142, 215	0
1	E	954/1045 (91%)	-0.82	1 (0%) 92 86	25, 70, 134, 209	0
1	F	959/1045 (91%)	-0.75	3 (0%) 90 79	26, 71, 139, 241	0
All	All	5742/6270 (91%)	-0.76	7 (0%) 92 86	25, 73, 140, 241	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	ASN	3.2
1	C	11	ASN	2.5
1	E	11	ASN	2.5
1	F	952	ARG	2.4
1	F	948	GLU	2.1
1	F	951	VAL	2.1
1	D	524	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	1101	1/1	0.98	0.03	108,108,108,108	0
2	ZN	A	1101	1/1	0.99	0.05	112,112,112,112	0
2	ZN	D	1101	1/1	0.99	0.06	111,111,111,111	1
2	ZN	E	1101	1/1	0.99	0.06	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.