WORLD WIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 04:31 AM EDT

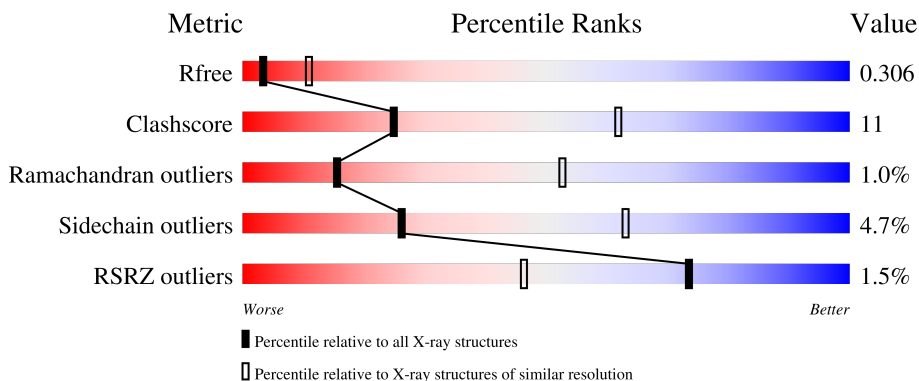|		
PDB ID	:	4K0J
Title	:	X-ray crystal structure of a heavy metal efflux pump, crystal form I
Authors	:	Pak, J.E.; Stroud, R.M.; Ngonlong Ekende, E.; Vandenbussche, G.; Center for Structures of Membrane Proteins (CSMP)
Deposited on	:	2013-04-04
Resolution	:	3.00 Å(reported)

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.
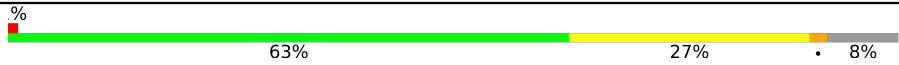
Metric	Percentile Ranks	Value
Rfree		0.306
Clashscore		11
Ramachandran outliers		1.0%
Sidechain outliers		4.7%
RSRZ outliers		1.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	2% 64% 26% • 8%
1	B	1045	% 65% 24% • 9%
1	C	1045	% 63% 26% • 8%
1	D	1045	2% 65% 25% • 8%
1	E	1045	% 64% 25% • 9%

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Mol	Chain	Length	Quality of chain
1	F	1045	63% 27% 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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 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)
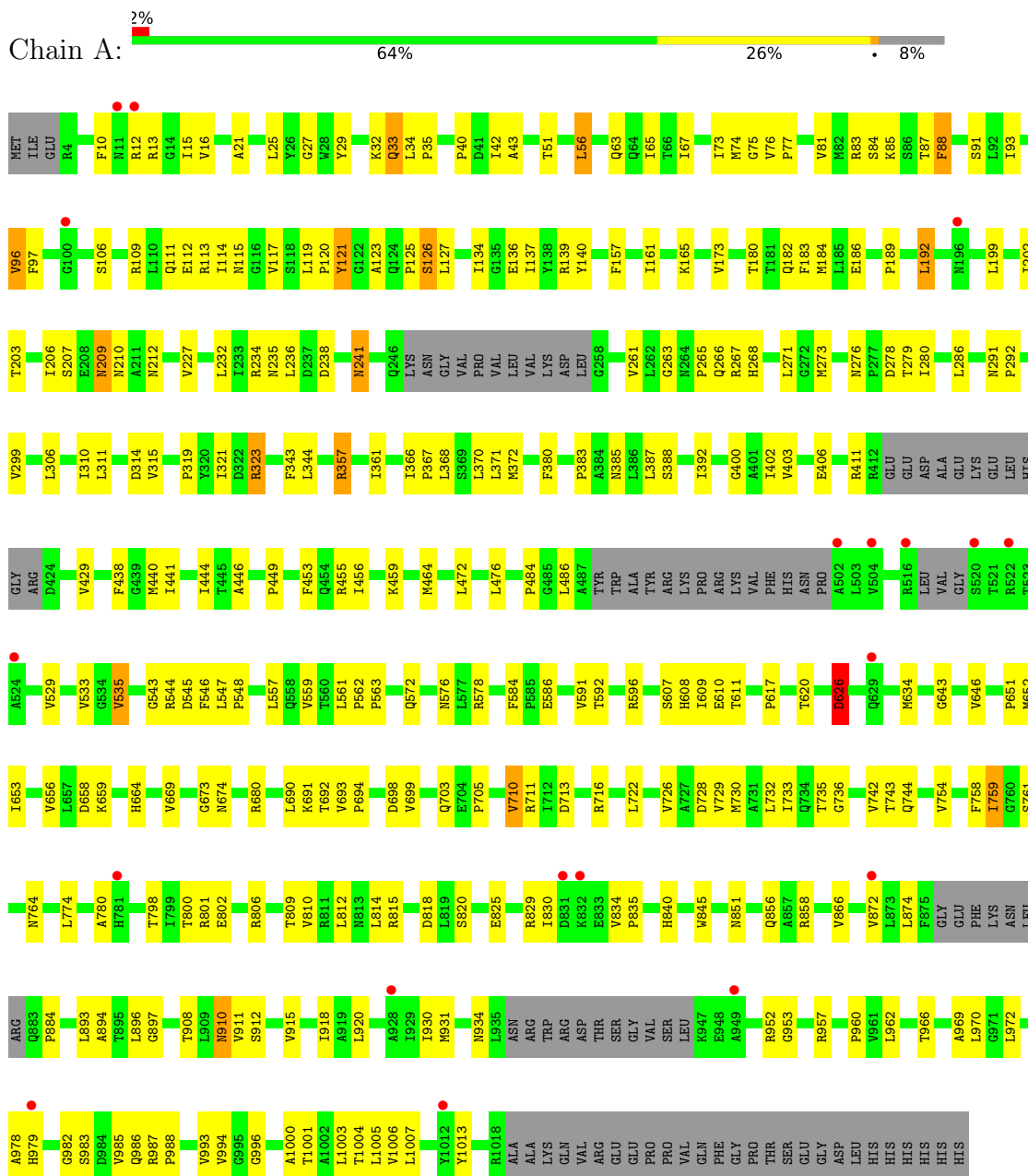
• Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)

Chain B:

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

Chain C:

• 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 F:
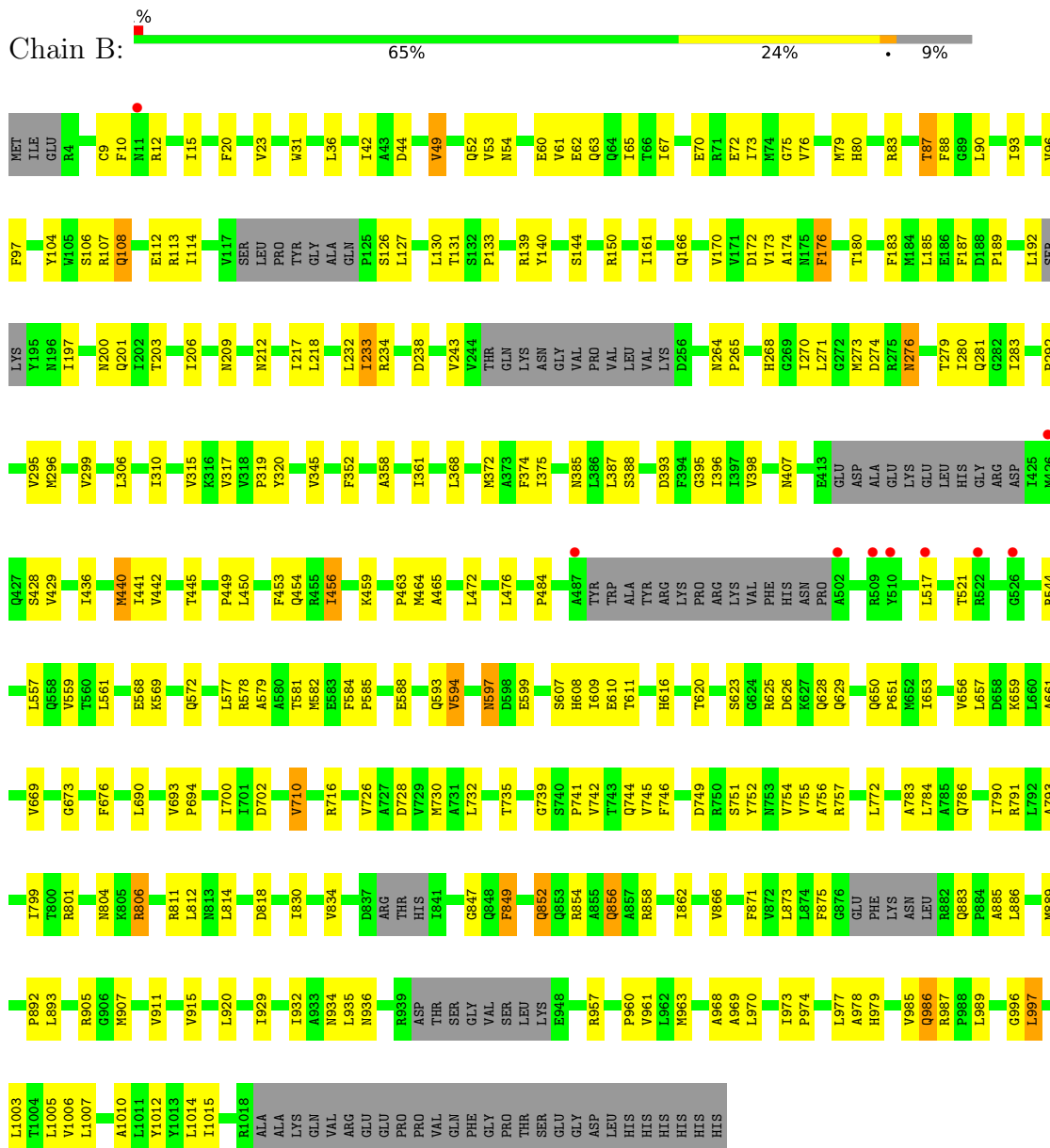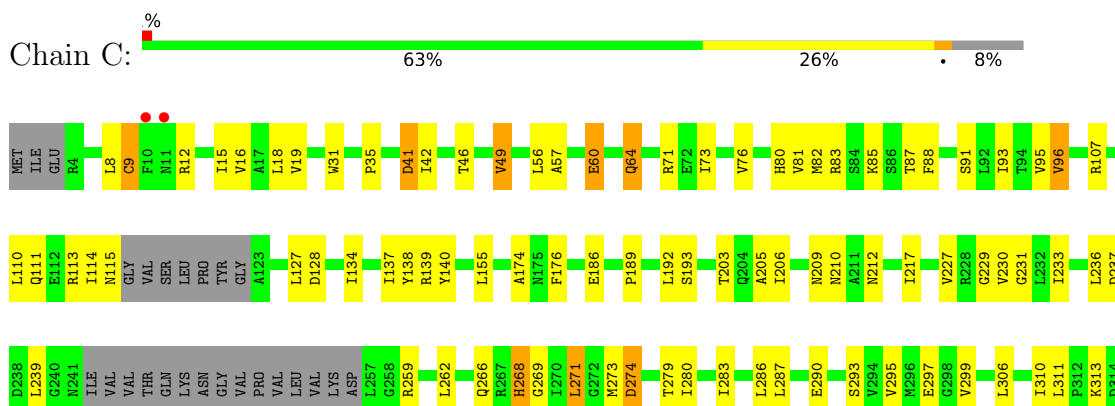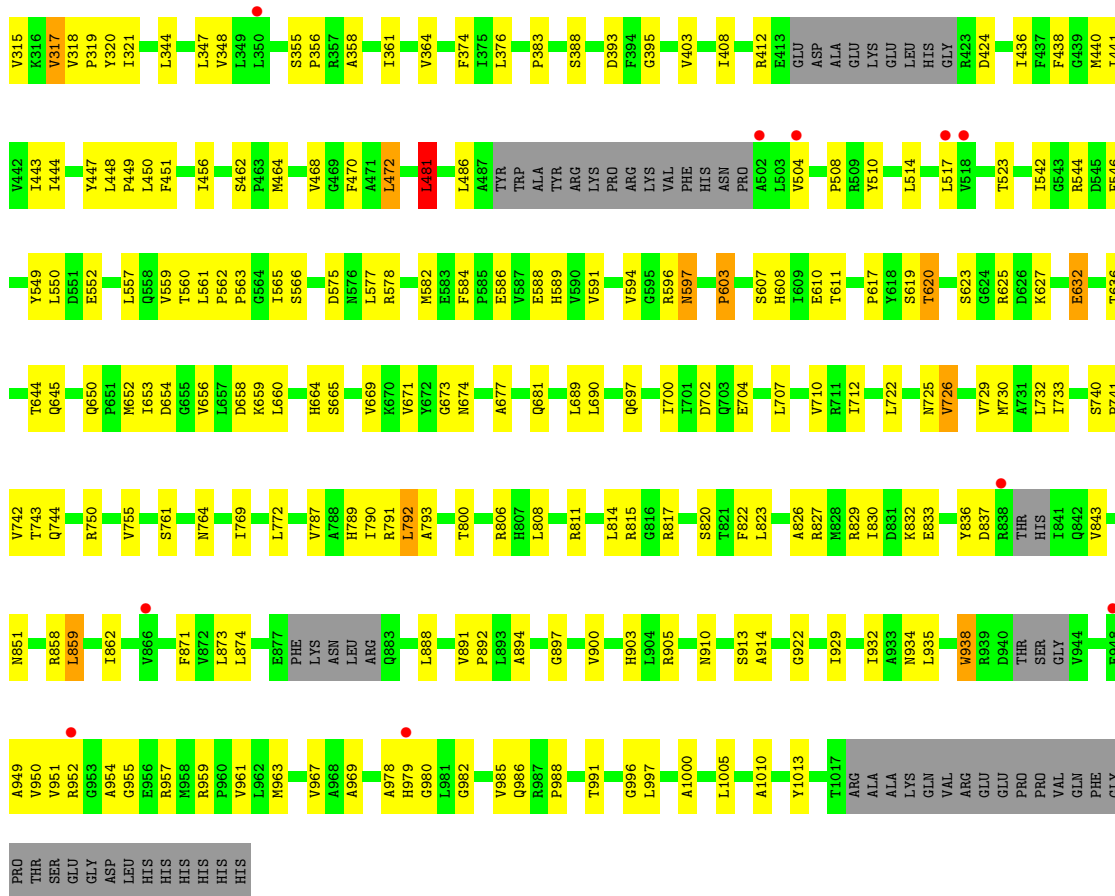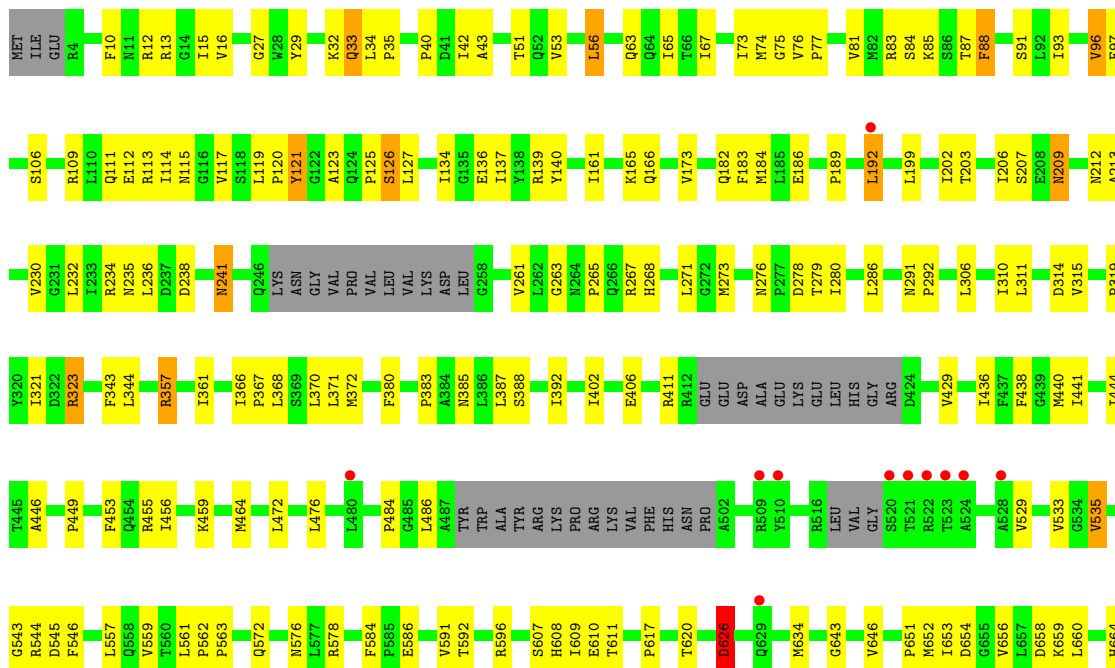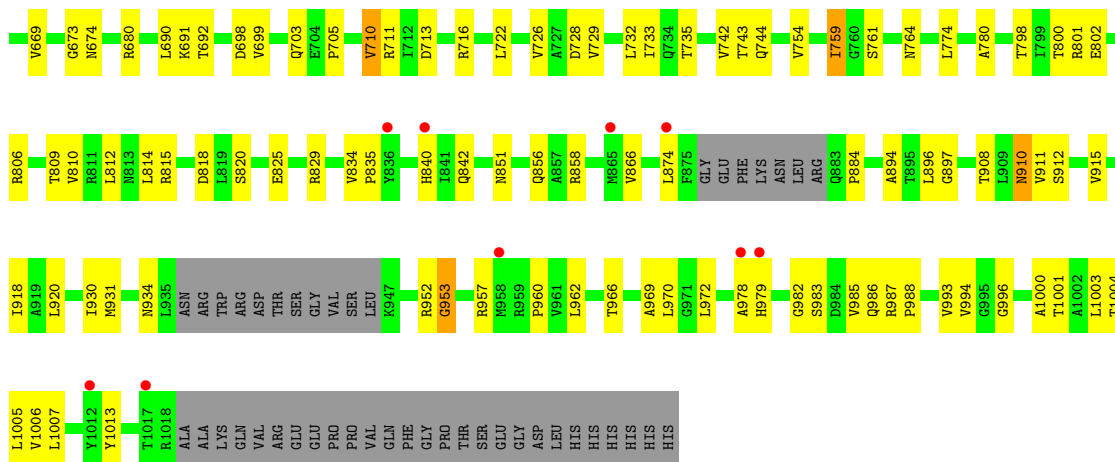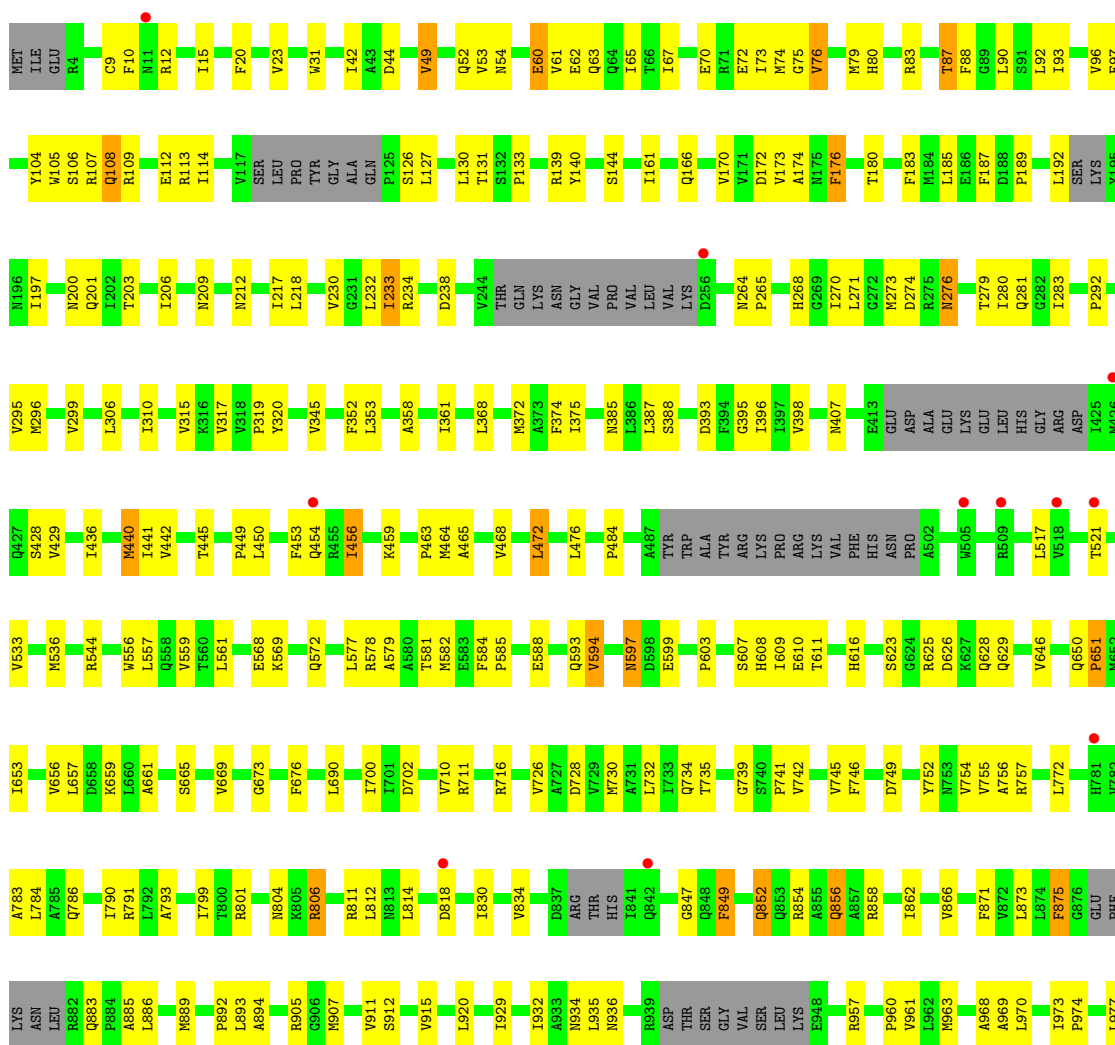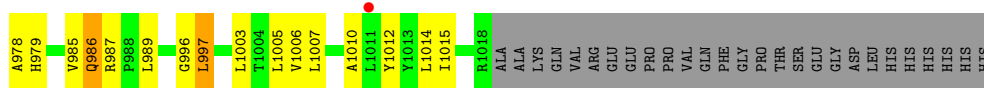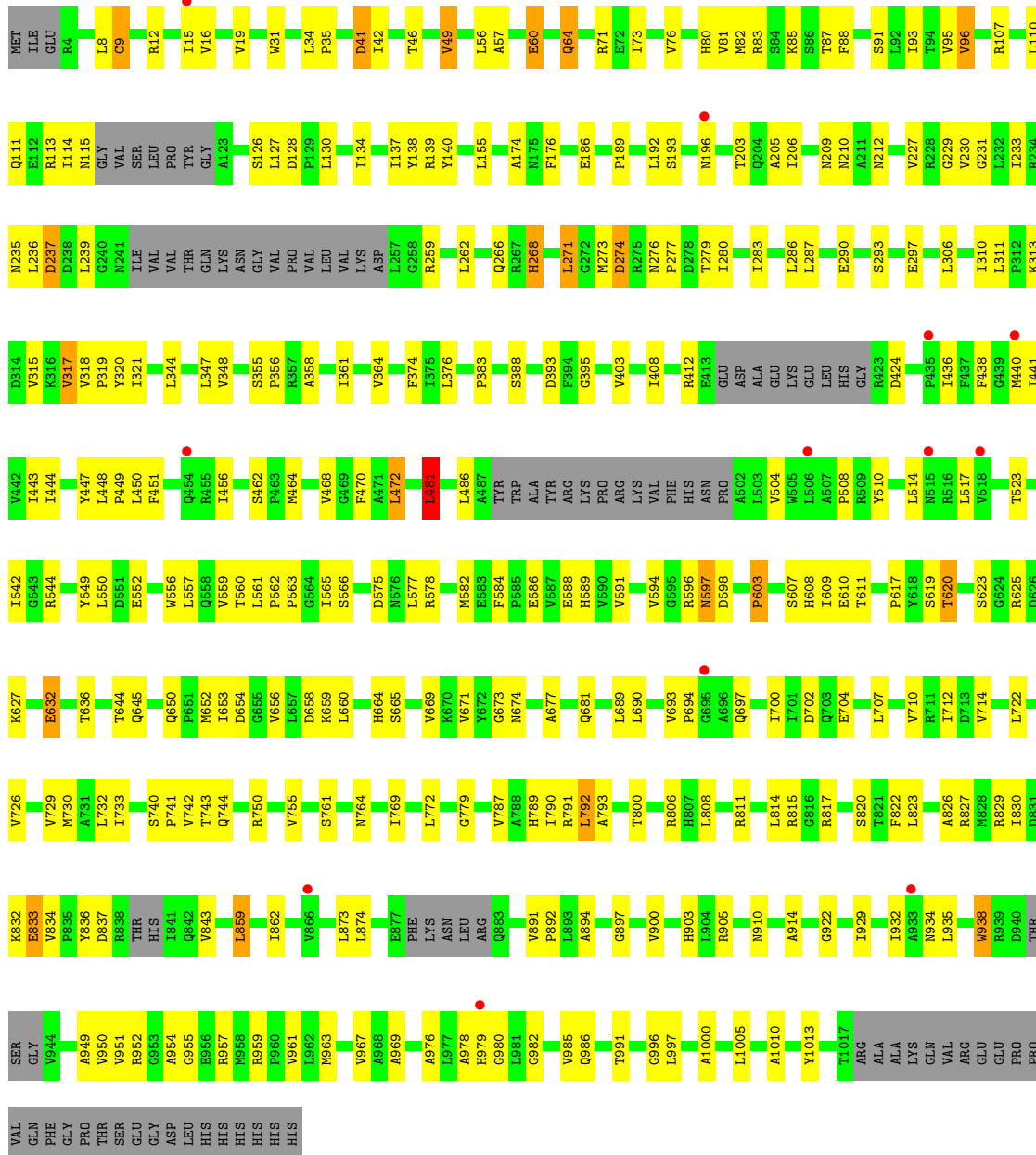
4 Data and refinement statistics (i)

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 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.98-3.00) 85.1 (19.98-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$<I/\sigma(I)>$ [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 , 0.306	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)	0.26 , 32.3	EDS
L-test for twinning[2]	$<|L|> = 0.34, <L^2> = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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	0.25	0/7461	0.46	0/10149
1	B	0.26	0/7436	0.46	0/10111
1	C	0.26	0/7480	0.46	0/10170
1	D	0.26	0/7461	0.46	0/10149
1	E	0.26	0/7436	0.46	0/10111
1	F	0.26	0/7480	0.46	0/10170
All	All	0.26	0/44754	0.46	0/60860

There are no bond length outliers.

There are no bond angle outliers.

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	168	0
1	B	7314	0	7588	155	0
1	C	7357	0	7626	173	0
1	D	7336	0	7607	161	0
1	E	7314	0	7588	167	0
1	F	7357	0	7626	175	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	966	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 (966) 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: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: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: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:B:407:ASN:ND2	1:B:428:SER:OG	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:NH1	1:A:713:ASP:OD2	2.32	0.60
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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:279:THR:OG1	1:D:280:ILE:N	2.36	0.55
1:E:276:ASN:HD21	1:E:279:THR:HB	1.71	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:126:SER:OG	1:D:127:LEU:N	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ARG:NH2	1:D:659:LYS:O	2.40	0.54
1:B:44:ASP:OD1	1:B:459:LYS:NZ	2.37	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:B:577:LEU:O	1:B:581:THR:OG1	2.18	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:352:PHE:HD2	1:B:963:MET:HE2	1.76	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: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:704:GLU:H	1:F:704:GLU:CD	2.14	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:352:PHE:HD2	1:E:963:MET:HE2	1.77	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:C:704:GLU:CD	1:C:704:GLU:H	2.13	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:A:279:THR:OG1	1:A:280:ILE:N	2.39	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
1:B:108:GLN:O	1:B:112:GLU:HG3	2.13	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:E:440:MET:HE3	1:E:441:ILE:HD12	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:241:ASN:OD1	1:A:241:ASN:N	2.46	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:C:743:THR:OG1	1:C:744:GLN:N	2.46	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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: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

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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	0.47
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: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
1:B:440:MET:HE3	1:B:441:ILE:HD12	1.96	0.46
1:E:73:ILE:HD11	1:E:114:ILE:HA	1.97	0.46
1:E:579:ALA:HA	1:E:582:MET:HE2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:87:THR:OG1	1:E:88:PHE:N	2.49	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: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:B:579:ALA:HA	1:B:582:MET:HE2	1.98	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
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:134:ILE:HB	1:D:652:MET:HE3	1.98	0.45
1:D:406:GLU:HG2	1:D:960:PRO:HB3	1.96	0.45
1:D:634:MET:HE3	1:D:634:MET:HB2	1.72	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:F:155:LEU:HD13	1:F:315:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:874:LEU:HB2	1:A:884:PRO:HB3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:88:PHE:HD2	1:F:596:ARG:HH22	1.67	0.43
1:A:634:MET:HE3	1:A:634:MET:HB2	1.74	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:912:SER:OG	1:E:985:VAL:O	2.22	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
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:42:ILE:O	1:B:459:LYS:NZ	2.47	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:126:SER:OG	1:E:127:LEU:N	2.49	0.43
1:E:133:PRO:HG2	1:E:656:VAL:HG12	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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:834:VAL:HA	1:A:835:PRO:HD3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:270:ILE:HB	1:B:594:VAL:HG13	2.01	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:730:MET:HE3	1:C:231:GLY:HA3	2.03	0.41
1:D:161:ILE:HG23	1:D:173:VAL:HB	2.02	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: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:1003:LEU:HG	1:A:1007:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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:533:VAL:HA	1:E:536:MET:HE2	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: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:166:GLN:HG2	1:E:74:MET:HE2	2.03	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: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: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%)	9	40
1	B	936/1045 (90%)	858 (92%)	76 (8%)	2 (0%)	47	82
1	C	943/1045 (90%)	850 (90%)	82 (9%)	11 (1%)	13	48
1	D	944/1045 (90%)	836 (89%)	93 (10%)	15 (2%)	9	40
1	E	936/1045 (90%)	860 (92%)	74 (8%)	2 (0%)	47	82
1	F	943/1045 (90%)	851 (90%)	81 (9%)	11 (1%)	13	48
All	All	5646/6270 (90%)	5092 (90%)	498 (9%)	56 (1%)	15	53

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 (i)

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%)	755 (96%)	32 (4%)	30	67
1	B	784/864 (91%)	746 (95%)	38 (5%)	25	62
1	C	789/864 (91%)	746 (95%)	43 (5%)	22	57
1	D	787/864 (91%)	756 (96%)	31 (4%)	32	69
1	E	784/864 (91%)	747 (95%)	37 (5%)	26	63
1	F	789/864 (91%)	747 (95%)	42 (5%)	22	58
All	All	4720/5184 (91%)	4497 (95%)	223 (5%)	26	63

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	56	LEU
1	A	96	VAL
1	A	126	SER
1	A	192	LEU
1	A	241	ASN
1	A	261	VAL
1	A	299	VAL
1	A	314	ASP
1	A	323	ARG
1	A	357	ARG
1	A	380	PHE
1	A	392	ILE
1	A	402	ILE
1	A	438	PHE
1	A	472	LEU
1	A	535	VAL
1	A	592	THR
1	A	626	ASP
1	A	680	ARG
1	A	692	THR
1	A	710	VAL
1	A	722	LEU
1	A	728	ASP
1	A	759	ILE
1	A	814	LEU
1	A	866	VAL

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Mol	Chain	Res	Type
1	A	910	ASN
1	A	930	ILE
1	A	931	MET
1	A	952	ARG
1	A	1013	TYR
1	B	49	VAL
1	B	60	GLU
1	B	63	GLN
1	B	87	THR
1	B	108	GLN
1	B	131	THR
1	B	150	ARG
1	B	170	VAL
1	B	176	PHE
1	B	180	THR
1	B	200	ASN
1	B	233	ILE
1	B	276	ASN
1	B	317	VAL
1	B	375	ILE
1	B	440	MET
1	B	456	ILE
1	B	472	LEU
1	B	544	ARG
1	B	594	VAL
1	B	597	ASN
1	B	620	THR
1	B	700	ILE
1	B	710	VAL
1	B	728	ASP
1	B	806	ARG
1	B	814	LEU
1	B	818	ASP
1	B	849	PHE
1	B	852	GLN
1	B	856	GLN
1	B	871	PHE
1	B	873	LEU
1	B	875	PHE
1	B	934	ASN
1	B	986	GLN
1	B	989	LEU

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Mol	Chain	Res	Type
1	B	997	LEU
1	C	9	CYS
1	C	49	VAL
1	C	56	LEU
1	C	60	GLU
1	C	64	GLN
1	C	91	SER
1	C	96	VAL
1	C	176	PHE
1	C	236	LEU
1	C	237	ASP
1	C	262	LEU
1	C	271	LEU
1	C	274	ASP
1	C	313	LYS
1	C	317	VAL
1	C	318	VAL
1	C	347	LEU
1	C	447	TYR
1	C	472	LEU
1	C	481	LEU
1	C	523	THR
1	C	550	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	700	ILE
1	C	710	VAL
1	C	726	VAL
1	C	740	SER
1	C	750	ARG
1	C	789	HIS
1	C	792	LEU
1	C	808	LEU
1	C	814	LEU
1	C	859	LEU
1	C	910	ASN
1	C	932	ILE

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Mol	Chain	Res	Type
1	C	938	TRP
1	C	1013	TYR
1	D	33	GLN
1	D	56	LEU
1	D	96	VAL
1	D	126	SER
1	D	192	LEU
1	D	241	ASN
1	D	261	VAL
1	D	314	ASP
1	D	323	ARG
1	D	357	ARG
1	D	380	PHE
1	D	392	ILE
1	D	402	ILE
1	D	438	PHE
1	D	472	LEU
1	D	535	VAL
1	D	592	THR
1	D	626	ASP
1	D	680	ARG
1	D	692	THR
1	D	710	VAL
1	D	722	LEU
1	D	728	ASP
1	D	759	ILE
1	D	814	LEU
1	D	866	VAL
1	D	910	ASN
1	D	930	ILE
1	D	931	MET
1	D	952	ARG
1	D	1013	TYR
1	E	49	VAL
1	E	60	GLU
1	E	63	GLN
1	E	76	VAL
1	E	87	THR
1	E	108	GLN
1	E	131	THR
1	E	170	VAL
1	E	176	PHE

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Mol	Chain	Res	Type
1	E	180	THR
1	E	200	ASN
1	E	233	ILE
1	E	276	ASN
1	E	317	VAL
1	E	375	ILE
1	E	440	MET
1	E	456	ILE
1	E	472	LEU
1	E	544	ARG
1	E	594	VAL
1	E	597	ASN
1	E	700	ILE
1	E	710	VAL
1	E	728	ASP
1	E	806	ARG
1	E	814	LEU
1	E	818	ASP
1	E	849	PHE
1	E	852	GLN
1	E	856	GLN
1	E	871	PHE
1	E	873	LEU
1	E	875	PHE
1	E	934	ASN
1	E	986	GLN
1	E	989	LEU
1	E	997	LEU
1	F	9	CYS
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	176	PHE
1	F	236	LEU
1	F	237	ASP
1	F	262	LEU
1	F	271	LEU
1	F	274	ASP
1	F	313	LYS

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Mol	Chain	Res	Type
1	F	317	VAL
1	F	318	VAL
1	F	347	LEU
1	F	447	TYR
1	F	472	LEU
1	F	481	LEU
1	F	523	THR
1	F	550	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	700	ILE
1	F	710	VAL
1	F	740	SER
1	F	750	ARG
1	F	789	HIS
1	F	792	LEU
1	F	808	LEU
1	F	814	LEU
1	F	859	LEU
1	F	910	ASN
1	F	932	ILE
1	F	938	TRP
1	F	1013	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	246	GLN
1	A	300	HIS
1	A	332	HIS
1	A	664	HIS
1	A	764	ASN
1	A	842	GLN
1	A	934	ASN
1	A	986	GLN
1	B	48	GLN

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Mol	Chain	Res	Type
1	B	52	GLN
1	B	54	ASN
1	B	166	GLN
1	B	201	GLN
1	B	264	ASN
1	B	276	ASN
1	B	300	HIS
1	B	407	ASN
1	B	572	GLN
1	B	597	ASN
1	B	753	ASN
1	B	771	ASN
1	B	852	GLN
1	B	936	ASN
1	C	111	GLN
1	C	182	GLN
1	C	204	GLN
1	C	268	HIS
1	C	289	ASN
1	C	753	ASN
1	C	764	ASN
1	C	804	ASN
1	C	848	GLN
1	C	934	ASN
1	D	33	GLN
1	D	246	GLN
1	D	300	HIS
1	D	332	HIS
1	D	664	HIS
1	D	764	ASN
1	D	842	GLN
1	D	934	ASN
1	D	986	GLN
1	E	48	GLN
1	E	52	GLN
1	E	54	ASN
1	E	166	GLN
1	E	201	GLN
1	E	264	ASN
1	E	276	ASN
1	E	300	HIS
1	E	407	ASN

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Mol	Chain	Res	Type
1	E	572	GLN
1	E	597	ASN
1	E	771	ASN
1	E	852	GLN
1	E	936	ASN
1	F	111	GLN
1	F	182	GLN
1	F	204	GLN
1	F	209	ASN
1	F	268	HIS
1	F	289	ASN
1	F	753	ASN
1	F	764	ASN
1	F	804	ASN
1	F	848	GLN
1	F	934	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	958/1045 (91%)	-0.26	19 (1%)	65	36	29, 77, 143, 215	0
1	B	954/1045 (91%)	-0.31	9 (0%)	84	63	27, 70, 135, 209	0
1	C	959/1045 (91%)	-0.30	12 (1%)	77	51	26, 71, 140, 241	0
1	D	958/1045 (91%)	-0.23	20 (2%)	63	34	29, 77, 142, 215	0
1	E	954/1045 (91%)	-0.30	12 (1%)	77	51	25, 70, 134, 209	0
1	F	959/1045 (91%)	-0.31	12 (1%)	77	51	26, 71, 139, 241	0
All	All	5742/6270 (91%)	-0.28	84 (1%)	73	46	25, 73, 140, 241	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	518	VAL	7.6
1	A	11	ASN	5.8
1	C	11	ASN	5.6
1	B	426	MET	5.2
1	D	978	ALA	4.8
1	A	522	ARG	4.7
1	C	517	LEU	4.4
1	D	836	TYR	4.4
1	B	487	ALA	4.3
1	A	832	LYS	4.2
1	C	948	GLU	4.1
1	A	504	VAL	4.0
1	A	100	GLY	4.0
1	A	831	ASP	3.9
1	A	520	SER	3.9
1	D	979	HIS	3.9
1	E	781	HIS	3.9
1	A	928	ALA	3.8
1	A	1012	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	952	ARG	3.8
1	D	522	ARG	3.7
1	E	11	ASN	3.7
1	D	874	LEU	3.6
1	E	509	ARG	3.5
1	F	979	HIS	3.4
1	D	840	HIS	3.3
1	D	524	ALA	3.3
1	D	510	TYR	3.3
1	F	454	GLN	3.3
1	A	12	ARG	3.2
1	E	521	THR	3.2
1	E	518	VAL	3.1
1	B	11	ASN	3.1
1	B	517	LEU	3.0
1	E	426	MET	3.0
1	D	480	LEU	3.0
1	F	196	ASN	2.9
1	C	979	HIS	2.9
1	D	520	SER	2.8
1	D	629	GLN	2.8
1	C	866	VAL	2.8
1	C	838	ARG	2.8
1	A	979	HIS	2.8
1	E	818	ASP	2.8
1	C	502	ALA	2.7
1	D	1017	THR	2.7
1	B	522	ARG	2.7
1	A	524	ALA	2.7
1	A	516	ARG	2.6
1	C	350	LEU	2.6
1	B	509	ARG	2.6
1	A	949	ALA	2.6
1	F	695	GLY	2.6
1	E	505	TRP	2.6
1	F	435	PRO	2.5
1	A	781	HIS	2.5
1	D	523	THR	2.5
1	E	842	GLN	2.5
1	F	518	VAL	2.5
1	F	440	MET	2.4
1	F	515	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	10	PHE	2.3
1	D	865	MET	2.3
1	A	196	ASN	2.3
1	E	454	GLN	2.3
1	D	192	LEU	2.3
1	E	1011	LEU	2.2
1	A	629	GLN	2.2
1	F	15	ILE	2.2
1	E	256	ASP	2.2
1	F	866	VAL	2.2
1	F	506	LEU	2.2
1	F	933	ALA	2.2
1	B	502	ALA	2.1
1	C	504	VAL	2.1
1	B	510	TYR	2.1
1	D	958	MET	2.1
1	D	1012	TYR	2.1
1	A	872	VAL	2.0
1	D	528	ALA	2.0
1	B	526	GLY	2.0
1	D	521	THR	2.0
1	A	502	ALA	2.0
1	D	509	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	ZN	B	1101	1/1	0.76	0.12	108,108,108,108	0
2	ZN	D	1101	1/1	0.87	0.11	111,111,111,111	1
2	ZN	E	1101	1/1	0.95	0.21	99,99,99,99	0
2	ZN	A	1101	1/1	0.97	0.23	112,112,112,112	0

6.5 Other polymers ⓘ

There are no such residues in this entry.