



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 PM GMT

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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

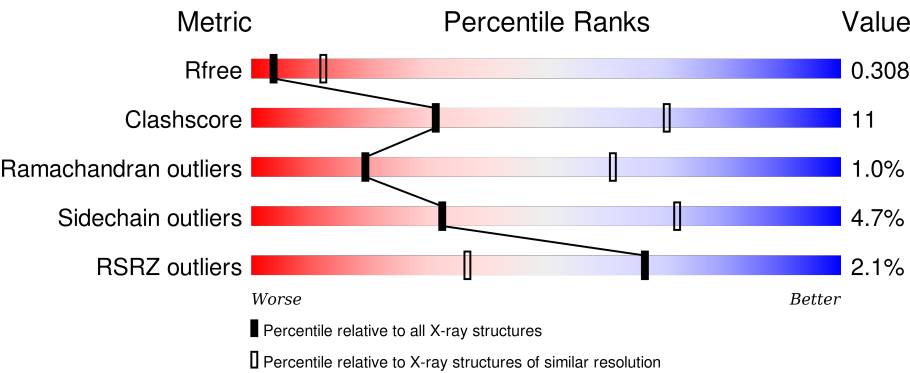
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div><div>2%</div><div></div><div>64%</div><div>26%</div><div>• 8%</div></div>
1	B	1045	<div><div>%</div><div></div><div>65%</div><div>24%</div><div>• 9%</div></div>
1	C	1045	<div><div>2%</div><div></div><div>63%</div><div>26%</div><div>• 8%</div></div>
1	D	1045	<div><div>3%</div><div></div><div>65%</div><div>25%</div><div>• 8%</div></div>
1	E	1045	<div><div>%</div><div></div><div>64%</div><div>25%</div><div>• 9%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	1045	<div><div></div><div>2%</div><div>63%</div><div>27%</div><div>• 8%</div></div>

## 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

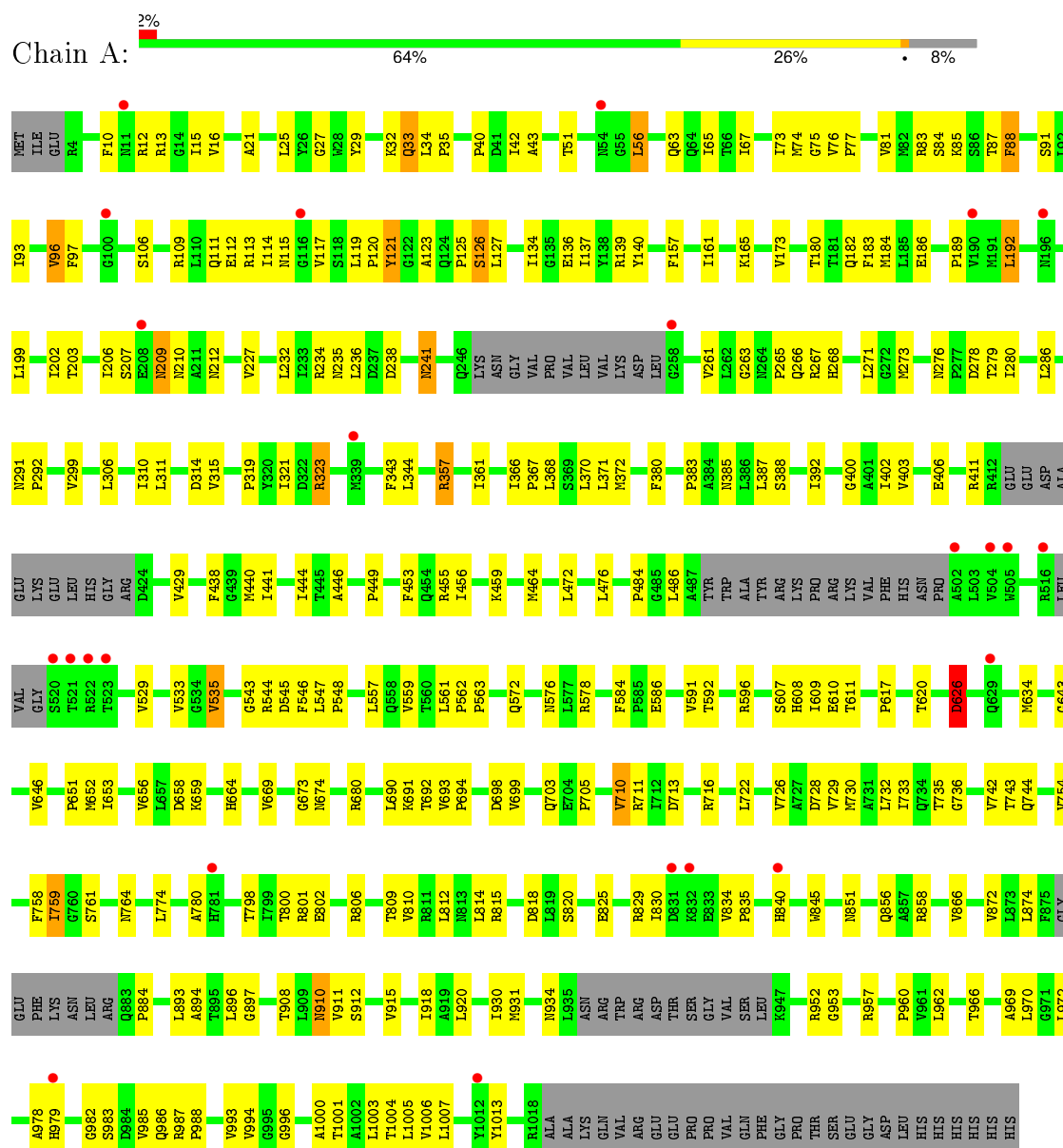
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

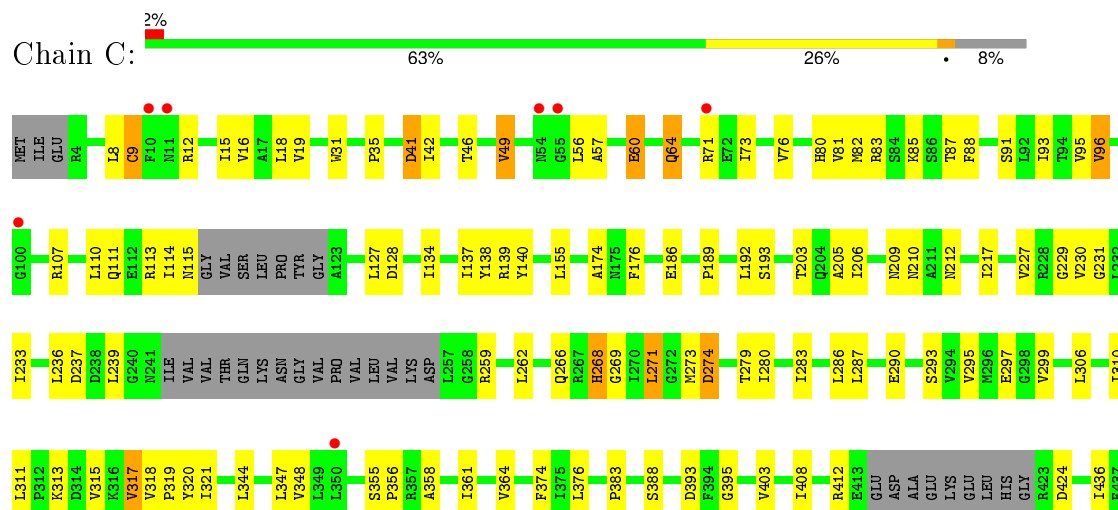
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0

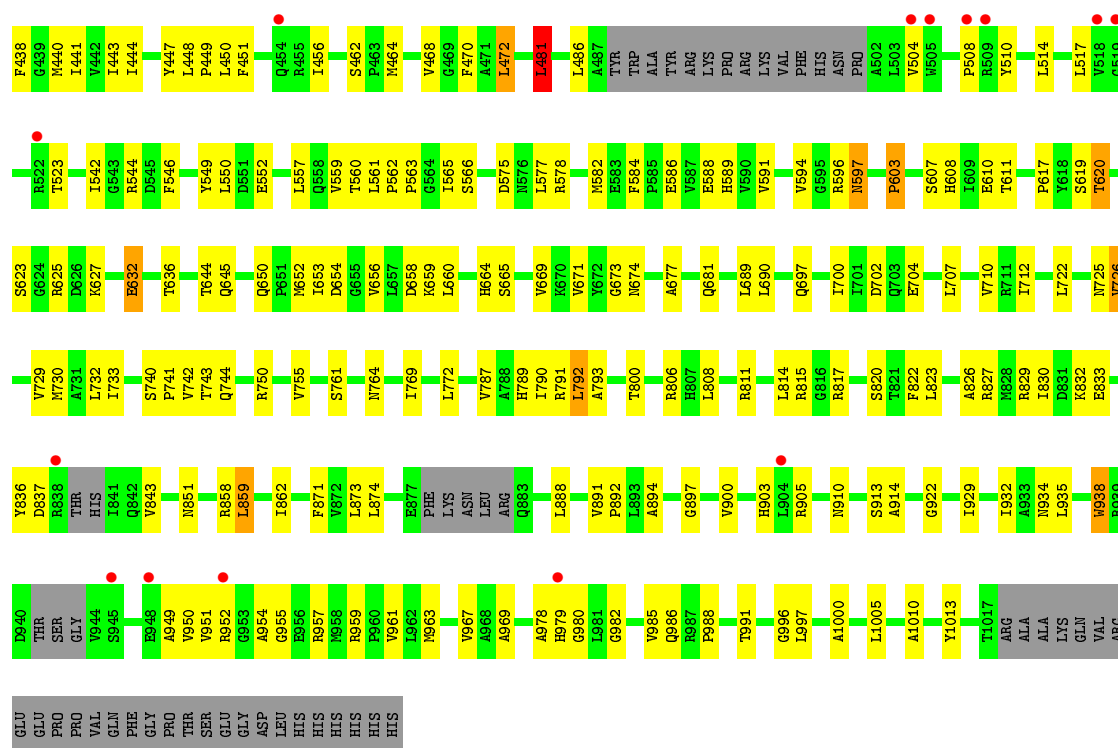
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

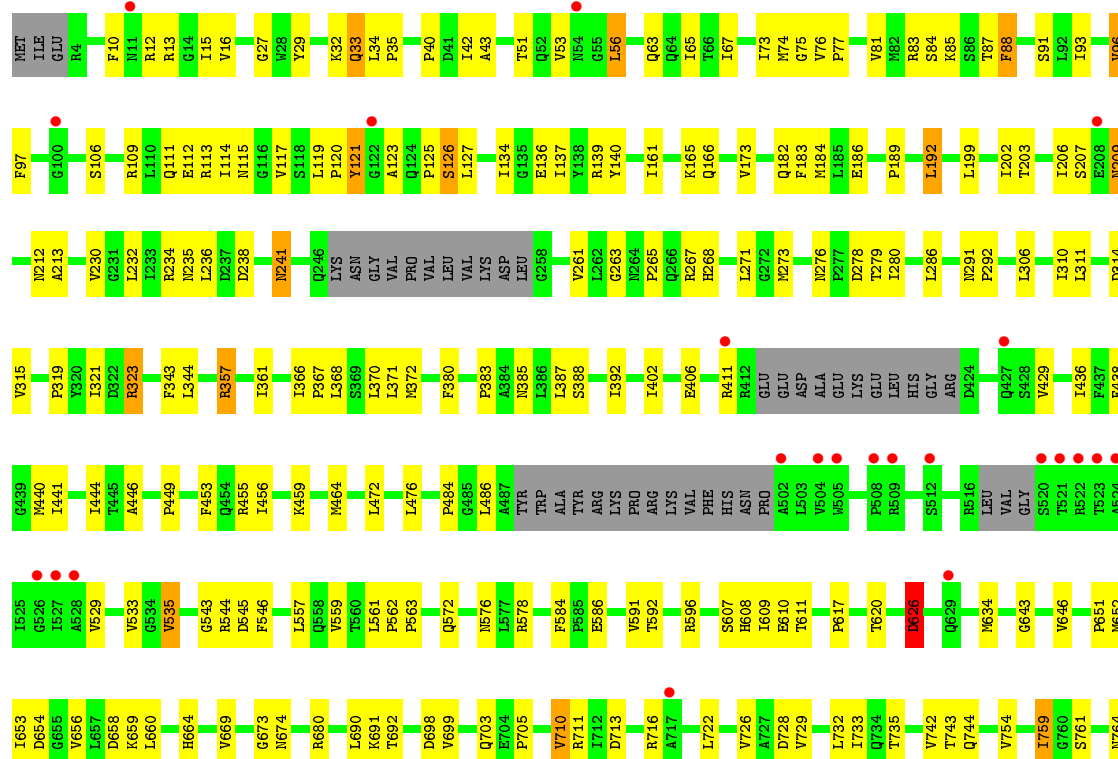
- Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)



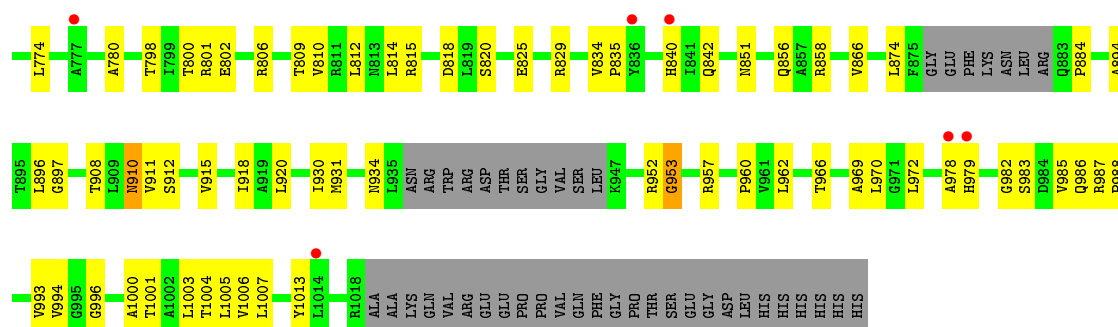




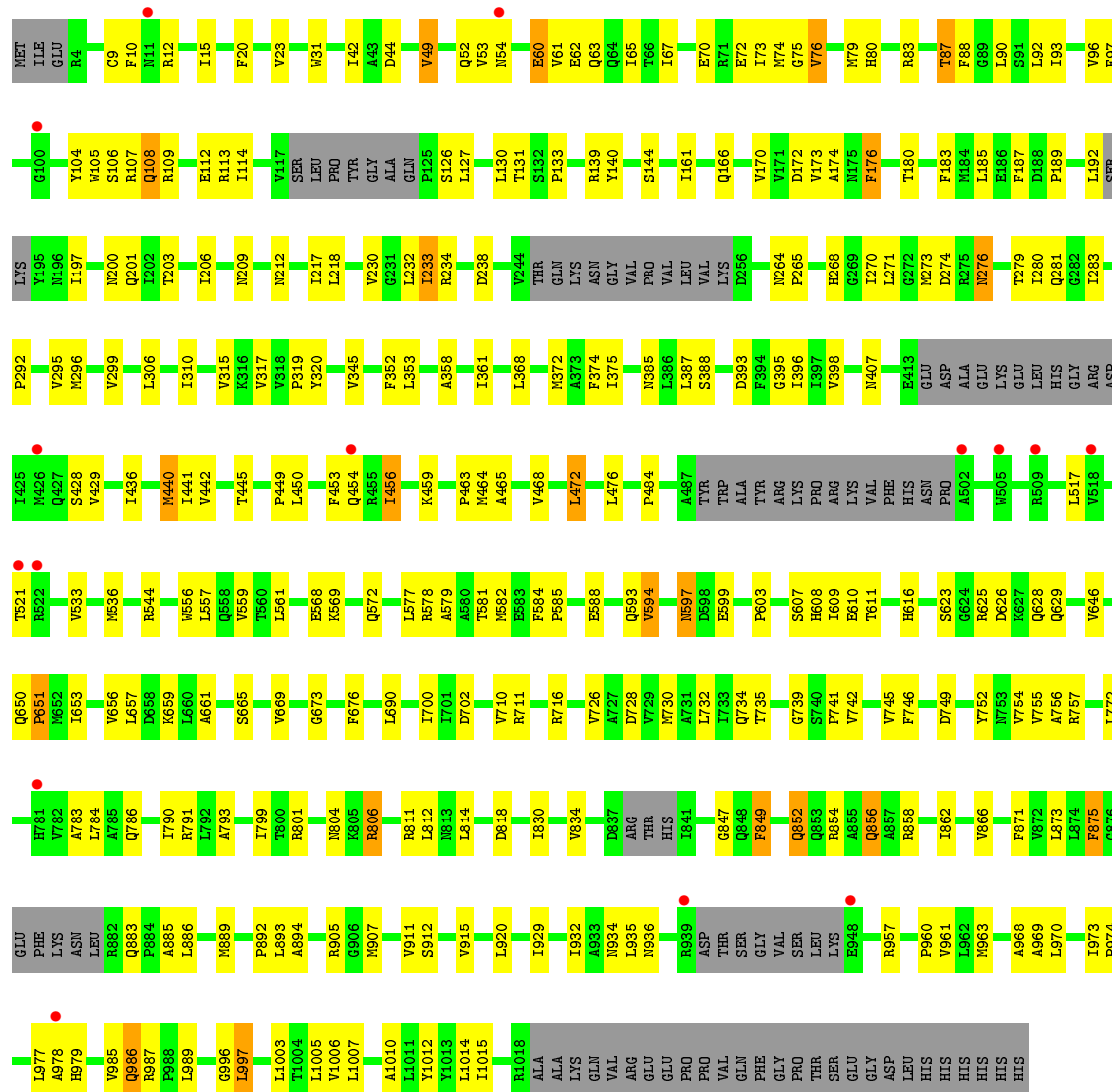
● Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)





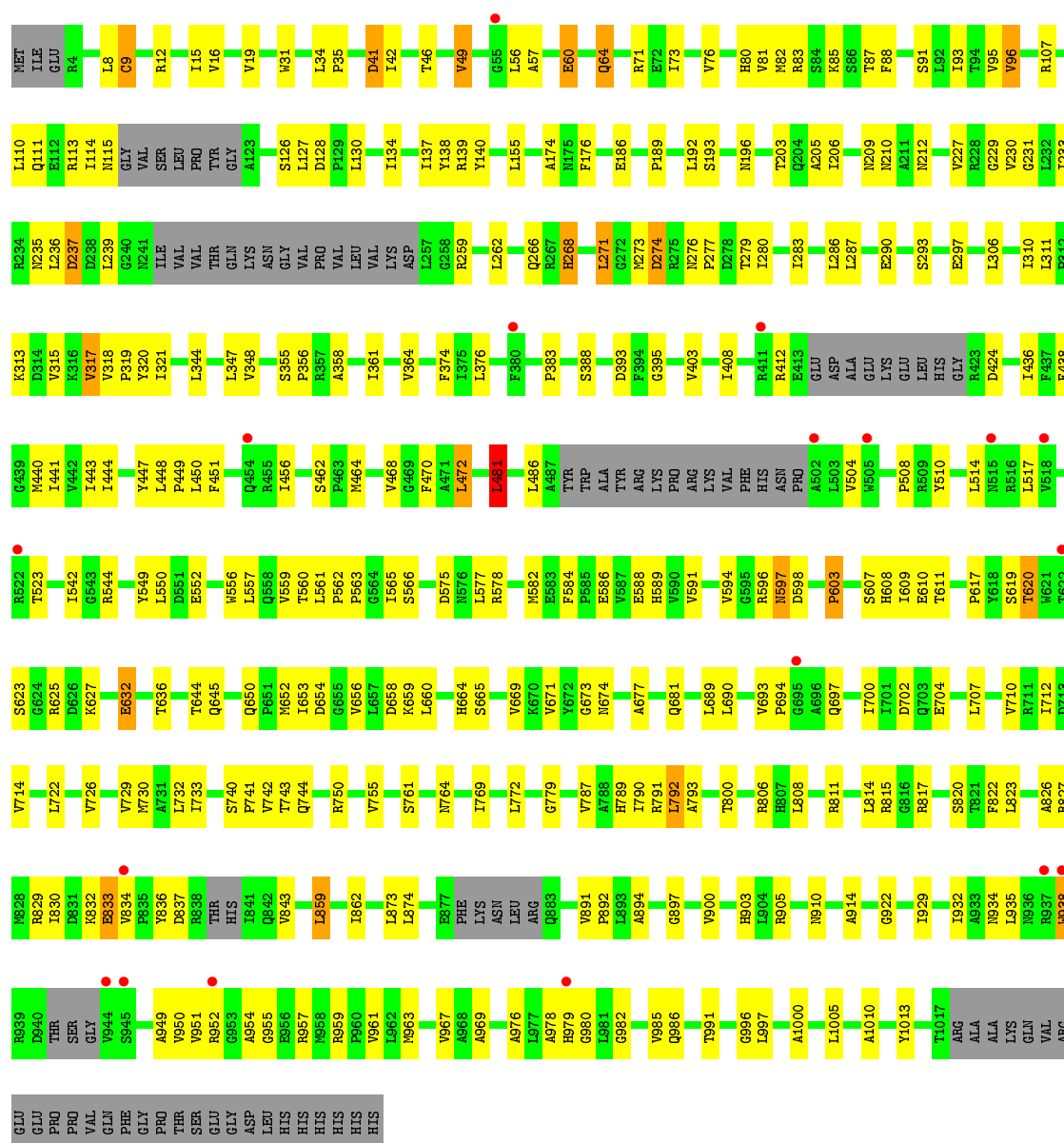


• Molecule 1: Heavy metal cation tricomponent efflux pump ZneA(CzcA-like)



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 95.9 (19.98-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.279 , 0.305 0.280 , 0.308	Depositor DCC
$R_{free}$ test set	1878 reflections (0.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 73.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	8 of 219455 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	44018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 [i](#)

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:B:83:ARG:NH2	1:B:659:LYS:O	2.21	0.73
1:A:111:GLN:O	1:A:115:ASN:ND2	2.19	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:E:62:GLU:OE1	1:E:801:ARG:NH1	2.24	0.70
1:A:119:LEU:HD12	1:A:125:PRO:HD3	1.72	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:D:559:VAL:HB	1:D:609:ILE:HB	1.76	0.68
1:C:205:ALA:O	1:C:209:ASN:ND2	2.25	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:D:81:VAL:HB	1:D:96:VAL:HG13	1.77	0.67
1:C:650:GLN:HB2	1:C:653:ILE:HG22	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:N	1:F:597:ASN:OD1	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:E:271:LEU:HD22	1:E:281:GLN:HB3	1.78	0.65
1:B:12:ARG:HG2	1:B:15:ILE:HB	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:F:443:ILE:HG13	1:F:922:GLY:HA3	1.79	0.64
1:D:711:ARG:NH1	1:D:713:ASP:OD2	2.30	0.64
1:D:306:LEU:HD23	1:D:310:ILE:HB	1.80	0.64
1:C:597:ASN:OD1	1:C:597:ASN:N	2.30	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:A:206:ILE:HG23	1:A:742:VAL:HG11	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:E:271:LEU:HD23	1:E:279:THR:HG23	1.80	0.63
1:D:12:ARG:HB3	1:D:16:VAL:HG13	1.80	0.63
1:A:674:ASN:O	1:A:806:ARG:NH2	2.31	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:C:203:THR:HA	1:C:206:ILE:HG22	1.81	0.62
1:F:544:ARG:HB2	1:F:820:SER:HB3	1.81	0.62
1:A:27:GLY:HA3	1:A:371:LEU:HB3	1.80	0.62
1:F:203:THR:HA	1:F:206:ILE:HG22	1.82	0.62
1:F:557:LEU:HB2	1:F:611:THR:HB	1.82	0.62
1:D:203:THR:HG21	1:D:735:THR:HG21	1.82	0.62
1:C:544:ARG:HB2	1:C:820:SER:HB3	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:F:306:LEU:HD23	1:F:310:ILE:HD12	1.82	0.61
1:D:626:ASP:OD1	1:D:626:ASP:N	2.33	0.61
1:D:76:VAL:HG12	1:D:113:ARG:HG3	1.82	0.61
1:B:716:ARG:HE	1:B:726:VAL:HG11	1.65	0.61
1:A:626:ASP:N	1:A:626:ASP:OD1	2.33	0.61
1:A:136:GLU:OE1	1:A:139:ARG:NH2	2.33	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:A:203:THR:HG21	1:A:735:THR:HG21	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:F:206:ILE:HD11	1:F:239:LEU:HD11	1.83	0.60
1:A:711:ARG:NH1	1:A:713:ASP:OD2	2.32	0.60
1:C:206:ILE:HD11	1:C:239:LEU:HD11	1.83	0.60
1:B:561:LEU:HB2	1:B:607:SER:O	2.00	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:F:233:ILE:HD11	1:F:239:LEU:HB2	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: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:E:456:ILE:HA	1:E:459:LYS:HD2	1.84	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:F:897:GLY:HA2	1:F:900:VAL:HG22	1.83	0.59
1:A:563:PRO:HB3	1:A:705:PRO:HD2	1.83	0.59
1:F:905:ARG:NH2	1:F:991:THR:OG1	2.32	0.59
1:E:232:LEU:HD23	1:E:234:ARG:HH12	1.67	0.59
1:E:801:ARG:NH2	1:E:804:ASN:OD1	2.36	0.59
1:E:440:MET:HG2	1:E:476:LEU:HD22	1.85	0.59
1:F:273:MET:HG3	1:F:591:VAL:HG22	1.85	0.59
1:B:52:GLN:NE2	1:B:599:GLU:O	2.35	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:985:VAL:HG13	1:B:986:GLN:HG3	1.86	0.58
1:B:440:MET:HG2	1:B:476:LEU:HD22	1.84	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:982:GLY:O	1:A:986:GLN:NE2	2.36	0.58
1:A:703:GLN:HE22	1:A:809:THR:H	1.52	0.58
1:A:235:ASN:ND2	1:A:238:ASP:OD1	2.36	0.58
1:E:702:ASP:OD1	1:E:811:ARG:NH1	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: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:801:ARG:NH2	1:B:804:ASN:OD1	2.37	0.57
1:B:183:PHE:HB2	1:B:754:VAL:HA	1.86	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: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:C:905:ARG:NH2	1:C:991:THR:OG1	2.31	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:D:557:LEU:HB2	1:D:611:THR:HB	1.87	0.57
1:A:343:PHE:HD2	1:A:344:LEU:HD22	1.70	0.57
1:F:982:GLY:O	1:F:986:GLN:NE2	2.37	0.57
1:D:51:THR:HB	1:D:91:SER:HB3	1.85	0.57
1:B:174:ALA:HB3	1:B:283:ILE:HB	1.86	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:E:76:VAL:HG23	1:E:79:MET:HB2	1.86	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: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:E:183:PHE:HB2	1:E:754:VAL:HA	1.87	0.56
1:A:83:ARG:NH2	1:A:659:LYS:O	2.39	0.56
1:D:535:VAL:HA	1:D:896:LEU:HD13	1.86	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: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:C:730:MET:HA	1:C:733:ILE:HD12	1.88	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:D:199:LEU:HD12	1:D:732:LEU:HA	1.87	0.56
1:C:712:ILE:HG12	1:C:790:ILE:HG13	1.87	0.56
1:B:739:GLY:HA3	1:B:757:ARG:HD3	1.88	0.56
1:E:174:ALA:HB3	1:E:283:ILE:HB	1.88	0.55
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: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:D:235:ASN:ND2	1:D:238:ASP:OD1	2.39	0.55
1:B:690:LEU:HD13	1:B:812:LEU:HD13	1.88	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:D:189:PRO:HA	1:D:192:LEU:HB2	1.89	0.55
1:C:741:PRO:HA	1:C:755:VAL:HG22	1.88	0.55
1:E:690:LEU:HD13	1:E:812:LEU:HD13	1.89	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: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:B:276:ASN:HD21	1:B:279:THR:HB	1.72	0.54
1:A:232:LEU:HD23	1:A:234:ARG:HH22	1.72	0.54
1:D:126:SER:OG	1:D:127:LEU:N	2.38	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:E:577:LEU:O	1:E:581:THR:OG1	2.18	0.54
1:A:1005:LEU:HD12	1:A:1006:VAL:HG23	1.90	0.54
1:C:440:MET:HA	1:C:443:ILE:HG22	1.90	0.54
1:B:279:THR:OG1	1:B:280:ILE:N	2.38	0.54
1:D:273:MET:HG3	1:D:591:VAL:HG22	1.90	0.54
1:F:891:VAL:HG23	1:F:892:PRO:HD3	1.89	0.54
1:C:702:ASP:OD1	1:C:811:ARG:NH1	2.41	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:726:VAL:O	1:E:730:MET:HG2	2.08	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

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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:E:608:HIS:HE1	1:E:610:GLU:HG3	1.74	0.53
1:B:577:LEU:O	1:B:581:THR:OG1	2.18	0.53
1:F:935:LEU:HD13	1:F:954:ALA:HB2	1.91	0.53
1:D:232:LEU:HD23	1:D:234:ARG:HH22	1.73	0.53
1:A:87:THR:HB	1:A:798:THR:HG22	1.89	0.53
1:C:73:ILE:HD11	1:C:114:ILE:HG22	1.91	0.53
1:B:49:VAL:HG13	1:B:93:ILE:HB	1.90	0.53
1:E:388:SER:HB3	1:E:464:MET:HB2	1.91	0.53
1:A:126:SER:OG	1:A:127:LEU:N	2.41	0.53
1:E:49:VAL:HG13	1:E:93:ILE:HB	1.91	0.53
1:B:388:SER:HB3	1:B:464:MET:HB2	1.91	0.53
1:D:1005:LEU:HD12	1:D:1006:VAL:HG23	1.91	0.53
1:B:140:TYR:HA	1:B:319:PRO:HA	1.89	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: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:C:891:VAL:HG23	1:C:892:PRO:HD3	1.91	0.52
1:B:449:PRO:HB3	1:B:862:ILE:HD13	1.89	0.52
1:F:836:TYR:HB3	1:F:837:ASP:HB2	1.90	0.52
1:B:429:VAL:HG21	1:B:484:PRO:HB3	1.90	0.52
1:A:969:ALA:HB1	1:A:994:VAL:HG13	1.92	0.52
1:E:849:PHE:HA	1:E:852:GLN:HB3	1.91	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: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:D:559:VAL:HG22	1:D:646:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:ASP:OD1	1:E:459:LYS:NZ	2.38	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:A:43:ALA:HB2	1:A:656:VAL:HG12	1.92	0.52
1:E:449:PRO:HD3	1:E:866:VAL:HG11	1.92	0.52
1:C:9:CYS:HB2	1:C:481:LEU:HD23	1.91	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:D:119:LEU:HB3	1:D:123:ALA:HB3	1.91	0.51
1:C:83:ARG:NH1	1:C:660:LEU:O	2.33	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:B:97:PHE:CZ	1:B:106:SER:HB2	2.44	0.51
1:F:949:ALA:HA	1:F:952:ARG:HB2	1.92	0.51
1:B:273:MET:HG3	1:B:274:ASP:H	1.73	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:F:376:LEU:HD12	1:F:470:PHE:HB3	1.91	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:D:87:THR:HB	1:D:798:THR:HG22	1.92	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: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:E:273:MET:HG3	1:E:274:ASP:H	1.74	0.51
1:D:761:SER:HA	1:D:764:ASN:ND2	2.24	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:B:858:ARG:O	1:B:862:ILE:HG13	2.10	0.51
1:D:698:ASP:OD2	1:D:815:ARG:NH1	2.32	0.51
1:F:697:GLN:HG2	1:F:815:ARG:CZ	2.41	0.51
1:C:376:LEU:HD12	1:C:470:PHE:HB3	1.93	0.51
1:C:575:ASP:OD1	1:C:578:ARG:NH2	2.42	0.51
1:B:557:LEU:HB3	1:B:611:THR:HB	1.93	0.51
1:F:87:THR:OG1	1:F:88:PHE:N	2.42	0.51
1:C:140:TYR:CD1	1:C:317:VAL:HG23	2.46	0.51
1:A:184:MET:HG3	1:A:263:GLY:HA3	1.92	0.51
1:C:448:LEU:HD22	1:C:451:PHE:HE2	1.76	0.51
1:A:761:SER:HA	1:A:764:ASN:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:GLN:OE1	1:B:320:TYR:OH	2.22	0.51
1:D:232:LEU:HD23	1:D:234:ARG:HH12	1.76	0.51
1:B:273:MET:O	1:B:578:ARG:NE	2.42	0.51
1:A:920:LEU:HD21	1:A:996:GLY:HA3	1.92	0.51
1:D:920:LEU:HD21	1:D:996:GLY:HA3	1.92	0.51
1:D:182:GLN:HG3	1:D:265:PRO:HD3	1.93	0.51
1:E:185:LEU:HB2	1:E:756:ALA:HA	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:A:559:VAL:HG22	1:A:646:VAL:HG22	1.92	0.50
1:F:575:ASP:OD1	1:F:578:ARG:NH2	2.40	0.50
1:A:267:ARG:NH1	1:A:278:ASP:OD2	2.45	0.50
1:C:41:ASP:HA	1:C:134:ILE:HD11	1.94	0.50
1:D:761:SER:HA	1:D:764:ASN:HD22	1.75	0.50
1:B:352:PHE:HD2	1:B:963:MET:HE2	1.76	0.50
1:F:448:LEU:HD22	1:F:451:PHE:HE2	1.76	0.50
1:C:697:GLN:HG2	1:C:815:ARG:CZ	2.41	0.50
1:D:969:ALA:HB1	1:D:994:VAL:HG13	1.93	0.50
1:A:653:ILE:HA	1:A:656:VAL:HG22	1.93	0.50
1:D:653:ILE:HA	1:D:656:VAL:HG22	1.93	0.50
1:A:761:SER:HA	1:A:764:ASN:ND2	2.26	0.50
1:D:669:VAL:HB	1:D:810:VAL:HB	1.93	0.50
1:F:817:ARG:HH11	1:F:822:PHE:HA	1.75	0.50
1:F:671:VAL:HG22	1:F:843:VAL:HG22	1.93	0.50
1:D:85:LYS:HE2	1:D:800:THR:HG22	1.94	0.50
1:A:182:GLN:HG3	1:A:265:PRO:HD3	1.93	0.50
1:A:87:THR:OG1	1:A:88:PHE:N	2.42	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:C:620:THR:O	1:C:620:THR:OG1	2.26	0.50
1:F:704:GLU:CD	1:F:704:GLU:H	2.14	0.50
1:F:358:ALA:HA	1:F:361:ILE:HG12	1.93	0.50
1:E:653:ILE:O	1:E:657:LEU:HG	2.12	0.50
1:A:669:VAL:HB	1:A:810:VAL:HB	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:B:53:VAL:HG21	1:B:65:ILE:HD13	1.94	0.50
1:A:202:ILE:O	1:A:206:ILE:HG22	2.12	0.49
1:F:403:VAL:HG21	1:F:436:ILE:HD11	1.93	0.49
1:C:46:THR:HG21	1:C:659:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ILE:O	1:D:206:ILE:HG22	2.12	0.49
1:B:749:ASP:HB2	1:C:71:ARG:HH22	1.75	0.49
1:F:189:PRO:HA	1:F:192:LEU:HD12	1.95	0.49
1:D:387:LEU:HB3	1:D:985:VAL:HG11	1.94	0.49
1:F:969:ALA:HB2	1:F:997:LEU:HD23	1.94	0.49
1:A:387:LEU:HB3	1:A:985:VAL:HG11	1.94	0.49
1:F:743:THR:OG1	1:F:744:GLN:N	2.45	0.49
1:A:729:VAL:HG22	1:A:774:LEU:HD11	1.94	0.49
1:D:357:ARG:HD2	1:D:357:ARG:H	1.77	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: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:D:35:PRO:HG2	1:D:383:PRO:HA	1.95	0.49
1:C:57:ALA:HA	1:C:88:PHE:HD1	1.77	0.49
1:E:352:PHE:HD2	1:E:963:MET:HE2	1.77	0.49
1:F:677:ALA:O	1:F:681:GLN:HG3	2.11	0.49
1:C:704:GLU:H	1:C:704:GLU:CD	2.13	0.49
1:C:560:THR:HB	1:C:645:GLN:HB2	1.94	0.49
1:C:358:ALA:HA	1:C:361:ILE:HG12	1.93	0.49
1:B:732:LEU:HD21	1:B:784:LEU:HD22	1.94	0.49
1:E:732:LEU:HD21	1:E:784:LEU:HD22	1.95	0.49
1:D:15:ILE:HG12	1:E:875:PHE:CE2	2.48	0.49
1:B:653:ILE:O	1:B:657:LEU:HG	2.12	0.49
1:B:67:ILE:HA	1:B:70:GLU:HG2	1.94	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:C:577:LEU:HD13	1:C:644:THR:HG21	1.95	0.49
1:B:176:PHE:CE1	1:B:593:GLN:HB3	2.47	0.49
1:D:311:LEU:HD13	1:D:315:VAL:HG12	1.94	0.49
1:B:393:ASP:OD1	1:B:396:ILE:N	2.44	0.49
1:F:140:TYR:CD1	1:F:317:VAL:HG23	2.48	0.49
1:F:393:ASP:O	1:F:395:GLY:N	2.43	0.49
1:D:267:ARG:NH1	1:D:278:ASP:OD2	2.46	0.49
1:E:440:MET:HE3	1:E:441:ILE:HD12	1.94	0.48
1:B:108:GLN:O	1:B:112:GLU:HG3	2.13	0.48
1:D:729:VAL:HG22	1:D:774:LEU:HD11	1.95	0.48
1:C:969:ALA:HB2	1:C:997:LEU:HD23	1.94	0.48
1:F:726:VAL:O	1:F:730:MET:HG2	2.13	0.48
1:B:306:LEU:HD23	1:B:310:ILE:HB	1.95	0.48
1:F:560:THR:HB	1:F:645:GLN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:20:PHE:HA	1:B:23:VAL:HG12	1.96	0.48
1:E:650:GLN:HB2	1:E:653:ILE:HG22	1.95	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:B:264:ASN:ND2	1:B:265:PRO:O	2.47	0.48
1:D:73:ILE:O	1:D:75:GLY:N	2.46	0.48
1:A:134:ILE:O	1:A:323:ARG:NH1	2.45	0.48
1:A:85:LYS:HE2	1:A:800:THR:HG22	1.95	0.48
1:B:791:ARG:HH21	1:B:793:ALA:HB2	1.79	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:C:510:TYR:CE2	1:C:955:GLY:HA2	2.49	0.48
1:C:438:PHE:HA	1:C:441:ILE:HG22	1.96	0.48
1:C:189:PRO:HA	1:C:192:LEU:HD12	1.94	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:A:441:ILE:HA	1:A:444:ILE:HG22	1.95	0.48
1:A:241:ASN:N	1:A:241:ASN:OD1	2.46	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: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:C:468:VAL:O	1:C:472:LEU:HB2	2.13	0.48
1:D:67:ILE:HA	1:D:801:ARG:HH12	1.79	0.48
1:E:784:LEU:HG	1:E:790:ILE:HD11	1.96	0.48
1:D:140:TYR:HA	1:D:319:PRO:HA	1.95	0.48
1:A:35:PRO:HG2	1:A:383:PRO:HA	1.96	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:F:57:ALA:HA	1:F:88:PHE:HD1	1.79	0.48
1:A:406:GLU:HG2	1:A:960:PRO:HB3	1.95	0.48
1:E:20:PHE:HA	1:E:23:VAL:HG12	1.95	0.48
1:B:61:VAL:HG11	1:B:90:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:ILE:HA	1:D:444:ILE:HG22	1.95	0.48
1:B:189:PRO:HA	1:B:192:LEU:HD12	1.94	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:A:357:ARG:HD2	1:A:357:ARG:H	1.78	0.48
1:E:172:ASP:OD1	1:E:173:VAL:N	2.41	0.47
1:C:791:ARG:HH21	1:C:793:ALA:HA	1.78	0.47
1:F:894:ALA:HA	1:F:1000:ALA:HB2	1.96	0.47
1:E:306:LEU:HD23	1:E:310:ILE:HB	1.95	0.47
1:A:698:ASP:O	1:A:812:LEU:HA	2.14	0.47
1:A:311:LEU:HD13	1:A:315:VAL:HG12	1.96	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:E:791:ARG:HH21	1:E:793:ALA:HB2	1.79	0.47
1:B:676:PHE:HZ	1:B:799:ILE:HG23	1.79	0.47
1:E:42:ILE:O	1:E:459:LYS:NZ	2.45	0.47
1:A:183:PHE:HB2	1:A:754:VAL:HA	1.96	0.47
1:B:653:ILE:HA	1:B:656:VAL:HG22	1.96	0.47
1:F:732:LEU:HD11	1:F:772:LEU:HD13	1.97	0.47
1:E:53:VAL:HG21	1:E:65:ILE:HD13	1.95	0.47
1:B:73:ILE:HD11	1:B:114:ILE:HA	1.96	0.47
1:D:690:LEU:HD22	1:D:812:LEU:HD13	1.97	0.47
1:B:784:LEU:HG	1:B:790:ILE:HD11	1.97	0.47
1:E:521:THR:HB	1:E:1014:LEU:HD22	1.95	0.47
1:D:698:ASP:O	1:D:812:LEU:HA	2.14	0.47
1:C:671:VAL:HG22	1:C:843:VAL:HG22	1.95	0.47
1:B:87:THR:OG1	1:B:88:PHE:N	2.47	0.47
1:D:691:LYS:HG3	1:D:699:VAL:HB	1.96	0.47
1:E:61:VAL:HG11	1:E:90:LEU:O	2.14	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:B:209:ASN:HB2	1:C:726:VAL:HG22	1.97	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:B:661:ALA:HB2	1:B:847:GLY:HA2	1.97	0.47
1:F:586:GLU:OE2	1:F:625:ARG:NH1	2.48	0.47
1:C:186:GLU:OE1	1:C:259:ARG:NH2	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:F:697:GLN:HG2	1:F:815:ARG:NH2	2.30	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:B:385:ASN:HB3	1:B:463:PRO:HG2	1.97	0.47
1:D:241:ASN:OD1	1:D:241:ASN:N	2.48	0.47
1:E:281:GLN:OE1	1:E:320:TYR:OH	2.23	0.47
1:A:67:ILE:HA	1:A:801:ARG:HH12	1.80	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:E:385:ASN:HB3	1:E:463:PRO:HG2	1.97	0.47
1:B:172:ASP:OD1	1:B:173:VAL:N	2.43	0.47
1:F:978:ALA:O	1:F:980:GLY:N	2.48	0.47
1:A:440:MET:HG3	1:A:476:LEU:HD22	1.96	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:B:893:LEU:HD22	1:B:1003:LEU:HD13	1.97	0.47
1:D:51:THR:HG21	1:D:65:ILE:HG21	1.97	0.46
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:F:620:THR:OG1	1:F:620:THR:O	2.27	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:D:617:PRO:HB2	1:D:620:THR:OG1	2.14	0.46
1:F:669:VAL:HG21	1:F:690:LEU:HD11	1.97	0.46
1:C:894:ALA:HA	1:C:1000:ALA:HB2	1.97	0.46
1:D:268:HIS:HB3	1:D:596:ARG:O	2.15	0.46
1:C:212:ASN:OD1	1:C:231:GLY:N	2.41	0.46
1:C:959:ARG:HD3	1:C:959:ARG:HA	1.74	0.46
1:B:440:MET:HE3	1:B:441:ILE:HD12	1.96	0.46
1:E:579:ALA:HA	1:E:582:MET:HE2	1.96	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:C:584:PHE:HB3	1:C:586:GLU:OE1	2.16	0.46
1:B:588:GLU:HB3	1:B:616:HIS:CE1	2.50	0.46
1:C:978:ALA:O	1:C:980:GLY:N	2.48	0.46
1:A:1001:THR:HA	1:A:1004:THR:HG22	1.98	0.46
1:E:144:SER:HB2	1:E:315:VAL:HG22	1.98	0.46
1:B:31:TRP:HB2	1:B:374:PHE:CD1	2.51	0.46
1:D:111:GLN:NE2	1:D:114:ILE:HD11	2.30	0.46
1:C:448:LEU:O	1:C:450:LEU:N	2.44	0.46
1:C:441:ILE:HG23	1:C:873:LEU:HD13	1.98	0.46
1:C:42:ILE:O	1:C:456:ILE:HG22	2.16	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:673:GLY:O	1:B:806:ARG:HB3	2.16	0.46
1:B:442:VAL:HA	1:B:445:THR:HG22	1.97	0.46
1:E:87:THR:OG1	1:E:88:PHE:N	2.49	0.46
1:C:673:GLY:O	1:C:806:ARG:HB2	2.16	0.46
1:C:552:GLU:OE2	1:C:652:MET:HB2	2.14	0.46
1:D:42:ILE:HG23	1:D:456:ILE:HB	1.98	0.46
1:A:212:ASN:ND2	1:A:232:LEU:HD22	2.31	0.46
1:A:51:THR:HG21	1:A:65:ILE:HG21	1.98	0.46
1:F:186:GLU:OE1	1:F:259:ARG:NH2	2.48	0.46
1:C:669:VAL:HG21	1:C:690:LEU:HD11	1.98	0.46
1:A:617:PRO:HB2	1:A:620:THR:OG1	2.15	0.46
1:F:436:ILE:HD13	1:F:436:ILE:HA	1.75	0.46
1:F:632:GLU:OE1	1:F:815:ARG:NH2	2.48	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:E:209:ASN:HB2	1:F:726:VAL:HG22	1.97	0.45
1:D:669:VAL:HG21	1:D:690:LEU:HD11	1.98	0.45
1:A:669:VAL:HG21	1:A:690:LEU:HD11	1.98	0.45
1:E:732:LEU:HD11	1:E:772:LEU:HD13	1.98	0.45
1:C:559:VAL:HG21	1:C:577:LEU:HD21	1.98	0.45
1:F:829:ARG:HA	1:F:832:LYS:HE3	1.98	0.45
1:B:579:ALA:HA	1:B:582:MET:HE2	1.98	0.45
1:B:217:ILE:HB	1:C:266:GLN:NE2	2.31	0.45
1:F:934:ASN:O	1:F:938:TRP:HB2	2.16	0.45
1:F:673:GLY:O	1:F:806:ARG:HB2	2.15	0.45
1:A:137:ILE:HD13	1:A:286:LEU:HB2	1.99	0.45
1:F:874:LEU:HD11	1:F:929:ILE:HD11	1.98	0.45
1:A:910:ASN:OD1	1:A:912:SER:HB3	2.16	0.45
1:D:733:ILE:HD13	1:F:229:GLY:HA3	1.99	0.45
1:C:35:PRO:HG2	1:C:383:PRO:HA	1.98	0.45
1:D:134:ILE:HB	1:D:652:MET:HE3	1.98	0.45
1:E:625:ARG:HG3	1:E:629:GLN:HB2	1.99	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:D:634:MET:HB2	1:D:634:MET:HE3	1.72	0.45
1:B:436:ILE:HD13	1:B:436:ILE:HA	1.84	0.45
1:F:155:LEU:HD13	1:F:315:VAL:HG11	1.99	0.45
1:C:107:ARG:NH2	1:C:128:ASP:O	2.47	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

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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:F:674:ASN:OD1	1:F:806:ARG:NH1	2.50	0.45
1:B:970:LEU:HG	1:B:973:ILE:HD12	1.99	0.45
1:E:673:GLY:O	1:E:806:ARG:HB3	2.16	0.45
1:E:588:GLU:HB3	1:E:616:HIS:CE1	2.51	0.45
1:D:953:GLY:O	1:D:957:ARG:N	2.44	0.45
1:F:8:LEU:O	1:F:12:ARG:HB2	2.16	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:F:542:ILE:HD13	1:F:903:HIS:CE1	2.52	0.45
1:E:929:ILE:HA	1:E:932:ILE:HG22	1.98	0.45
1:D:710:VAL:HG13	1:F:227:VAL:HG22	1.99	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:691:LYS:HG3	1:A:699:VAL:HB	1.98	0.45
1:A:268:HIS:HB3	1:A:596:ARG:O	2.16	0.45
1:A:203:THR:O	1:A:207:SER:OG	2.22	0.45
1:C:155:LEU:HD13	1:C:315:VAL:HG11	1.98	0.45
1:C:791:ARG:NH2	1:C:792:LEU:O	2.50	0.45
1:D:910:ASN:OD1	1:D:912:SER:HB3	2.17	0.45
1:D:109:ARG:O	1:D:112:GLU:HB2	2.17	0.45
1:F:212:ASN:OD1	1:F:231:GLY:N	2.40	0.45
1:A:872:VAL:HG13	1:C:18:LEU:HD23	1.99	0.45
1:D:543:GLY:HA3	1:D:908:THR:HG22	1.99	0.45
1:C:542:ILE:HD13	1:C:903:HIS:CE1	2.52	0.45
1:F:424:ASP:OD1	1:F:424:ASP:N	2.50	0.45
1:D:436:ILE:HA	1:D:436:ILE:HD13	1.85	0.45
1:C:320:TYR:CD1	1:C:321:ILE:HG13	2.52	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:F:320:TYR:CD1	1:F:321:ILE:HG13	2.51	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:C:829:ARG:HA	1:C:832:LYS:HE3	1.98	0.44
1:C:934:ASN:O	1:C:938:TRP:HB2	2.16	0.44
1:B:144:SER:HB2	1:B:315:VAL:HG22	1.98	0.44
1:F:35:PRO:HG2	1:F:383:PRO:HA	1.99	0.44
1:A:33:GLN:HE21	1:A:33:GLN:HB2	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:GLU:OE1	1:C:815:ARG:NH2	2.49	0.44
1:F:791:ARG:NH2	1:F:792:LEU:O	2.50	0.44
1:C:674:ASN:HA	1:C:806:ARG:HG3	1.99	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:A:918:ILE:HA	1:A:918:ILE:HD13	1.81	0.44
1:C:874:LEU:HD11	1:C:929:ILE:HD11	1.98	0.44
1:A:139:ARG:HB2	1:A:321:ILE:HB	2.00	0.44
1:F:441:ILE:HG23	1:F:873:LEU:HD13	1.97	0.44
1:E:746:PHE:CD1	1:F:64:GLN:HG2	2.52	0.44
1:E:653:ILE:HA	1:E:656:VAL:HG22	2.00	0.44
1:A:56:LEU:HD21	1:C:212:ASN:O	2.18	0.44
1:F:654:ASP:OD2	1:F:664:HIS:ND1	2.50	0.44
1:F:897:GLY:HA3	1:F:996:GLY:HA2	2.00	0.44
1:C:588:GLU:HG2	1:C:589:HIS:CD2	2.53	0.44
1:C:514:LEU:HB3	1:C:951:VAL:HG22	1.99	0.44
1:F:408:ILE:O	1:F:412:ARG:HB3	2.17	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:D:236:LEU:HD23	1:D:236:LEU:H	1.82	0.44
1:A:73:ILE:HD11	1:A:114:ILE:HG22	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:B:1006:VAL:HG12	1:B:1007:LEU:HD23	2.00	0.44
1:F:905:ARG:NH1	1:F:976:ALA:O	2.43	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:F:42:ILE:O	1:F:456:ILE:HG22	2.18	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:B:9:CYS:SG	1:B:10:PHE:N	2.91	0.44
1:A:825:GLU:O	1:A:829:ARG:HG3	2.18	0.44
1:E:9:CYS:SG	1:E:10:PHE:N	2.91	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: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:B:957:ARG:HH11	1:B:960:PRO:HG3	1.83	0.44
1:F:355:SER:HA	1:F:356:PRO:HD2	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:137:ILE:HD13	1:D:286:LEU:HB2	2.00	0.44
1:E:957:ARG:HH11	1:E:960:PRO:HG3	1.83	0.44
1:D:918:ILE:HA	1:D:918:ILE:HD13	1.80	0.44
1:A:726:VAL:HB	1:C:209:ASN:HB2	2.00	0.43
1:D:56:LEU:HD21	1:F:212:ASN:O	2.17	0.43
1:B:584:PHE:HA	1:B:585:PRO:HD3	1.83	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: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:B:450:LEU:HA	1:B:453:PHE:CE2	2.53	0.43
1:C:436:ILE:HD13	1:C:436:ILE:HA	1.74	0.43
1:B:970:LEU:HA	1:B:973:ILE:HG13	2.00	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:F:562:PRO:HG2	1:F:565:ILE:HG13	1.99	0.43
1:E:977:LEU:HB3	1:E:979:HIS:NE2	2.33	0.43
1:A:673:GLY:HA2	1:A:840:HIS:HB2	2.00	0.43
1:F:210:ASN:OD1	1:F:233:ILE:HG22	2.18	0.43
1:D:985:VAL:O	1:D:988:PRO:HD2	2.17	0.43
1:D:366:ILE:HB	1:D:367:PRO:HD3	2.01	0.43
1:E:1006:VAL:HG12	1:E:1007:LEU:HD23	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:A:366:ILE:HB	1:A:367:PRO:HD3	2.00	0.43
1:E:345:VAL:HG11	1:E:398:VAL:HG21	2.00	0.43
1:C:654:ASP:OD2	1:C:664:HIS:ND1	2.52	0.43
1:C:206:ILE:CG2	1:C:742:VAL:HG11	2.49	0.43
1:E:911:VAL:O	1:E:915:VAL:HG23	2.18	0.43
1:D:361:ILE:HG23	1:D:486:LEU:HD12	2.00	0.43
1:B:977:LEU:HB3	1:B:979:HIS:NE2	2.33	0.43
1:A:361:ILE:HG23	1:A:486:LEU:HD12	2.01	0.43
1:E:450:LEU:HD11	1:E:915:VAL:HG13	2.00	0.43
1:A:874:LEU:HB2	1:A:884:PRO:HB3	2.00	0.43
1:F:823:LEU:O	1:F:827:ARG:HB3	2.19	0.43
1:F:588:GLU:HG2	1:F:589:HIS:CD2	2.54	0.43
1:D:165:LYS:HE2	1:D:165:LYS:HB3	1.81	0.43
1:C:562:PRO:HG2	1:C:565:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ASN:OD1	1:C:233:ILE:HG22	2.19	0.43
1:F:88:PHE:HD2	1:F:596:ARG:HH22	1.67	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:E:166:GLN:HE21	1:E:166:GLN:HB3	1.65	0.43
1:D:368:LEU:O	1:D:372:MET:HG3	2.19	0.43
1:E:912:SER:OG	1:E:985:VAL:O	2.22	0.43
1:C:897:GLY:HA3	1:C:996:GLY:HA2	2.01	0.43
1:F:791:ARG:HE	1:F:793:ALA:HB2	1.83	0.43
1:B:973:ILE:N	1:B:974:PRO:HD2	2.33	0.43
1:B:625:ARG:HG3	1:B:629:GLN:HB2	1.99	0.43
1:C:268:HIS:HB2	1:C:269:GLY:H	1.70	0.43
1:A:634:MET:HB2	1:A:634:MET:HE3	1.74	0.43
1:A:716:ARG:CZ	1:A:726:VAL:HG21	2.49	0.43
1:F:597:ASN:HB2	1:F:598:ASP:H	1.56	0.43
1:E:970:LEU:HA	1:E:973:ILE:HG13	2.00	0.43
1:F:654:ASP:OD1	1:F:664:HIS:HB3	2.19	0.43
1:B:693:VAL:HA	1:B:694:PRO:HD3	1.94	0.43
1:A:368:LEU:O	1:A:372:MET:HG3	2.19	0.43
1:F:449:PRO:HB2	1:F:862:ILE:HG23	2.01	0.43
1:F:80:HIS:ND1	1:F:81:VAL:HG23	2.34	0.43
1:A:236:LEU:H	1:A:236:LEU:HD23	1.83	0.43
1:C:287:LEU:HD23	1:C:290:GLU:HG3	2.01	0.43
1:B:42:ILE:O	1:B:459:LYS:NZ	2.47	0.43
1:E:133:PRO:HG2	1:E:656:VAL:HG12	2.01	0.43
1:C:674:ASN:OD1	1:C:806:ARG:NH1	2.52	0.43
1:B:932:ILE:HA	1:B:935:LEU:HB2	2.00	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:A:186:GLU:HB3	1:A:759:ILE:HG13	2.00	0.43
1:F:561:LEU:HB2	1:F:607:SER:O	2.19	0.43
1:F:950:VAL:O	1:F:954:ALA:HB3	2.19	0.42
1:C:689:LEU:HD12	1:C:830:ILE:HD13	2.01	0.42
1:A:529:VAL:O	1:A:533:VAL:HG23	2.19	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:A:411:ARG:HD2	1:A:411:ARG:HA	1.87	0.42
1:E:139:ARG:HB3	1:E:320:TYR:CZ	2.53	0.42
1:F:206:ILE:CG2	1:F:742:VAL:HG11	2.49	0.42
1:E:742:VAL:N	1:E:754:VAL:O	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:852:GLN:NE2	1:E:856:GLN:HE21	2.18	0.42
1:F:448:LEU:O	1:F:450:LEU:N	2.45	0.42
1:C:704:GLU:OE2	1:C:704:GLU:N	2.51	0.42
1:F:81:VAL:HB	1:F:96:VAL:HG13	2.00	0.42
1:D:561:LEU:HB2	1:D:607:SER:O	2.19	0.42
1:E:889:MET:O	1:E:892:PRO:HD2	2.18	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:B:886:LEU:HD11	1:B:1015:ILE:HG21	2.00	0.42
1:D:911:VAL:O	1:D:915:VAL:HG23	2.20	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:A:710:VAL:HG13	1:C:227:VAL:HG22	2.01	0.42
1:A:227:VAL:HG22	1:B:710:VAL:HG13	2.01	0.42
1:E:230:VAL:O	1:F:714:VAL:HG22	2.19	0.42
1:B:295:VAL:O	1:B:299:VAL:HG23	2.19	0.42
1:B:75:GLY:O	1:B:113:ARG:NH2	2.52	0.42
1:A:711:ARG:NH1	1:C:230:VAL:HG21	2.34	0.42
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.82	0.42
1:A:972:LEU:HD12	1:A:993:VAL:HG11	2.02	0.42
1:C:444:ILE:HD11	1:C:472:LEU:HB3	2.02	0.42
1:F:212:ASN:HD21	1:F:230:VAL:HG13	1.84	0.42
1:D:1003:LEU:HG	1:D:1007:LEU:HD13	2.02	0.42
1:C:449:PRO:HB2	1:C:862:ILE:HG23	2.02	0.42
1:E:741:PRO:HA	1:E:755:VAL:HG22	2.01	0.42
1:F:293:SER:O	1:F:297:GLU:HG3	2.18	0.42
1:C:517:LEU:HD22	1:C:1010:ALA:HB2	2.02	0.42
1:A:743:THR:OG1	1:A:744:GLN:N	2.53	0.42
1:C:563:PRO:HB2	1:C:707:LEU:HD21	2.00	0.42
1:E:161:ILE:HG12	1:E:173:VAL:HG11	2.02	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:C:504:VAL:O	1:C:508:PRO:HD3	2.20	0.42
1:B:345:VAL:HG11	1:B:398:VAL:HG21	2.01	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:B:139:ARG:HB3	1:B:320:TYR:CZ	2.54	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:B:749:ASP:HB2	1:C:71:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:GLU:O	1:B:572:GLN:HG3	2.18	0.42
1:A:29:TYR:O	1:A:33:GLN:NE2	2.53	0.42
1:E:973:ILE:N	1:E:974:PRO:HD2	2.33	0.42
1:A:366:ILE:O	1:A:370:LEU:HG	2.20	0.42
1:F:287:LEU:HD23	1:F:290:GLU:HG3	2.01	0.42
1:A:834:VAL:HA	1:A:835:PRO:HD3	1.77	0.42
1:B:961:VAL:HG11	1:B:1005:LEU:HD21	2.02	0.42
1:A:165:LYS:HE2	1:A:165:LYS:HB3	1.80	0.42
1:A:12:ARG:O	1:A:16:VAL:HG22	2.20	0.42
1:D:83:ARG:HG2	1:D:802:GLU:OE2	2.19	0.42
1:E:852:GLN:HE22	1:E:856:GLN:HE21	1.67	0.42
1:C:293:SER:O	1:C:297:GLU:HG3	2.20	0.42
1:D:40:PRO:HG3	1:D:385:ASN:OD1	2.20	0.42
1:F:196:ASN:HD21	1:F:779:GLY:HA2	1.85	0.42
1:C:355:SER:HA	1:C:356:PRO:HD2	1.90	0.42
1:D:529:VAL:O	1:D:533:VAL:HG23	2.19	0.42
1:E:665:SER:OG	1:E:811:ARG:HB2	2.20	0.42
1:F:279:THR:OG1	1:F:280:ILE:N	2.52	0.42
1:A:344:LEU:HB3	1:A:970:LEU:HG	2.02	0.42
1:E:206:ILE:HG12	1:E:742:VAL:HG11	2.02	0.42
1:F:87:THR:HG21	1:F:603:PRO:HB2	2.02	0.42
1:B:885:ALA:O	1:B:889:MET:HG2	2.20	0.42
1:D:186:GLU:HB3	1:D:759:ILE:HG13	2.01	0.42
1:A:291:ASN:HA	1:A:292:PRO:HD3	1.89	0.42
1:D:10:PHE:O	1:D:13:ARG:HG3	2.20	0.42
1:A:109:ARG:O	1:A:112:GLU:HB2	2.19	0.42
1:E:353:LEU:HA	1:E:353:LEU:HD12	1.85	0.42
1:C:858:ARG:HD3	1:C:858:ARG:HA	1.87	0.42
1:D:73:ILE:HD11	1:D:114:ILE:HG22	2.02	0.42
1:C:279:THR:OG1	1:C:280:ILE:N	2.50	0.42
1:B:852:GLN:NE2	1:B:856:GLN:HE21	2.18	0.42
1:A:920:LEU:HD13	1:A:993:VAL:HA	2.01	0.42
1:D:972:LEU:HD12	1:D:993:VAL:HG11	2.02	0.42
1:C:729:VAL:O	1:C:732:LEU:HB3	2.20	0.42
1:D:56:LEU:HD23	1:D:56:LEU:HA	1.90	0.42
1:C:268:HIS:H	1:C:268:HIS:CD2	2.37	0.42
1:D:658:ASP:HB2	1:D:664:HIS:CD2	2.54	0.42
1:E:745:VAL:HG13	1:E:752:TYR:HB2	2.02	0.42
1:C:963:MET:O	1:C:967:VAL:HG22	2.20	0.42
1:B:54:ASN:HD21	1:B:268:HIS:CE1	2.37	0.42
1:D:230:VAL:HG21	1:E:711:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ILE:HA	1:B:201:GLN:NE2	2.35	0.42
1:E:978:ALA:HA	1:E:987:ARG:HD3	2.02	0.42
1:F:268:HIS:H	1:F:268:HIS:CD2	2.37	0.42
1:E:75:GLY:O	1:E:113:ARG:NH2	2.53	0.41
1:D:12:ARG:O	1:D:16:VAL:HG22	2.20	0.41
1:A:456:ILE:HD11	1:A:546:PHE:CE1	2.55	0.41
1:D:234:ARG:HB2	1:D:238:ASP:OD2	2.20	0.41
1:E:450:LEU:HA	1:E:453:PHE:CE2	2.54	0.41
1:C:87:THR:HG21	1:C:603:PRO:HB2	2.01	0.41
1:A:56:LEU:HD11	1:A:121:TYR:CE2	2.55	0.41
1:D:834:VAL:HA	1:D:835:PRO:HD3	1.77	0.41
1:A:161:ILE:HG23	1:A:173:VAL:HB	2.02	0.41
1:E:105:TRP:O	1:E:109:ARG:HG2	2.19	0.41
1:A:658:ASP:HB2	1:A:664:HIS:CD2	2.54	0.41
1:F:126:SER:OG	1:F:127:LEU:N	2.52	0.41
1:B:669:VAL:HG21	1:B:690:LEU:HD11	2.01	0.41
1:D:56:LEU:HD11	1:D:121:TYR:CE2	2.55	0.41
1:F:517:LEU:HD22	1:F:1010:ALA:HB2	2.02	0.41
1:E:197:ILE:HA	1:E:201:GLN:NE2	2.36	0.41
1:D:874:LEU:HB2	1:D:884:PRO:HB3	2.01	0.41
1:B:270:ILE:HB	1:B:594:VAL:HG13	2.01	0.41
1:F:514:LEU:HB3	1:F:951:VAL:HG22	2.00	0.41
1:D:34:LEU:HD12	1:D:34:LEU:HA	1.92	0.41
1:E:60:GLU:HG2	1:E:60:GLU:H	1.59	0.41
1:D:139:ARG:HB2	1:D:321:ILE:HB	2.02	0.41
1:A:234:ARG:HB2	1:A:238:ASP:OD2	2.20	0.41
1:A:83:ARG:HG2	1:A:802:GLU:OE2	2.20	0.41
1:F:565:ILE:HG22	1:F:566:SER:O	2.20	0.41
1:A:693:VAL:HA	1:A:694:PRO:HD3	1.88	0.41
1:B:978:ALA:HA	1:B:987:ARG:HD3	2.03	0.41
1:B:358:ALA:O	1:B:361:ILE:HG22	2.20	0.41
1:F:836:TYR:HA	1:F:837:ASP:HA	1.92	0.41
1:C:88:PHE:HD2	1:C:596:ARG:HH22	1.69	0.41
1:C:791:ARG:HE	1:C:793:ALA:HB2	1.84	0.41
1:E:358:ALA:HA	1:E:361:ILE:HG22	2.02	0.41
1:A:10:PHE:O	1:A:13:ARG:HG3	2.19	0.41
1:E:292:PRO:O	1:E:296:MET:HB2	2.20	0.41
1:F:563:PRO:HB2	1:F:707:LEU:HD21	2.01	0.41
1:C:344:LEU:O	1:C:348:VAL:HG23	2.20	0.41
1:B:830:ILE:O	1:B:834:VAL:HG22	2.20	0.41
1:F:693:VAL:HA	1:F:694:PRO:HD3	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:A:1006:VAL:HG12	1:A:1007:LEU:HD12	2.02	0.41
1:D:897:GLY:HA3	1:D:996:GLY:HA2	2.02	0.41
1:B:745:VAL:HG13	1:B:752:TYR:HB2	2.02	0.41
1:F:276:ASN:HA	1:F:277:PRO:HD3	1.86	0.41
1:B:741:PRO:HA	1:B:755:VAL:HG22	2.01	0.41
1:A:266:GLN:NE2	1:C:217:ILE:HB	2.36	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:E:830:ILE:O	1:E:834:VAL:HG22	2.20	0.41
1:B:187:PHE:HE2	1:B:756:ALA:HB1	1.85	0.41
1:F:957:ARG:HA	1:F:957:ARG:HD3	1.73	0.41
1:C:938:TRP:HZ3	1:C:952:ARG:HH21	1.69	0.41
1:F:444:ILE:HD11	1:F:472:LEU:HB3	2.01	0.41
1:D:654:ASP:OD1	1:D:664:HIS:HB3	2.21	0.41
1:B:358:ALA:HA	1:B:361:ILE:HG22	2.02	0.41
1:E:358:ALA:O	1:E:361:ILE:HG22	2.20	0.41
1:E:920:LEU:HD21	1:E:996:GLY:HA3	2.03	0.41
1:F:963:MET:O	1:F:967:VAL:HG22	2.21	0.41
1:D:842:GLN:HB3	1:D:842:GLN:HE21	1.62	0.41
1:C:273:MET:O	1:C:578:ARG:NE	2.54	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:B:161:ILE:HG12	1:B:173:VAL:HG11	2.03	0.41
1:E:885:ALA:O	1:E:889:MET:HG2	2.21	0.41
1:B:744:GLN:NE2	1:B:751:SER:OG	2.40	0.41
1:E:961:VAL:HG11	1:E:1005:LEU:HD21	2.02	0.41
1:D:584:PHE:HB3	1:D:586:GLU:OE1	2.20	0.41
1:A:446:ALA:O	1:A:449:PRO:HD2	2.21	0.41
1:A:40:PRO:HG3	1:A:385:ASN:OD1	2.21	0.41
1:D:608:HIS:CE1	1:D:610:GLU:HG3	2.56	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:F:826:ALA:O	1:F:830:ILE:HG12	2.21	0.41
1:A:561:LEU:HB2	1:A:607:SER:O	2.21	0.41
1:E:92:LEU:HD21	1:E:603:PRO:HB3	2.03	0.41
1:A:276:ASN:ND2	1:A:279:THR:HB	2.35	0.41
1:A:1003:LEU:HG	1:A:1007:LEU:HD13	2.02	0.41
1:D:83:ARG:NH1	1:D:660:LEU:O	2.49	0.41
1:C:617:PRO:HB2	1:C:620:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:LEU:HD13	1:C:951:VAL:HA	2.03	0.41
1:C:80:HIS:ND1	1:C:81:VAL:HG23	2.36	0.41
1:F:689:LEU:HD12	1:F:830:ILE:HD13	2.02	0.41
1:D:291:ASN:HA	1:D:292:PRO:HD3	1.90	0.41
1:E:468:VAL:O	1:E:472:LEU:HB2	2.21	0.41
1:D:29:TYR:O	1:D:33:GLN:NE2	2.54	0.41
1:C:859:LEU:HD21	1:C:914:ALA:HB1	2.03	0.41
1:C:138:TYR:CE2	1:C:319:PRO:HB3	2.56	0.41
1:B:243:VAL:HB	1:C:725:ASN:OD1	2.20	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: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:D:716:ARG:CZ	1:D:726:VAL:HG21	2.51	0.41
1:A:584:PHE:HB3	1:A:586:GLU:OE1	2.21	0.41
1:A:32:LYS:HA	1:A:32:LYS:HD3	1.89	0.41
1:F:273:MET:O	1:F:578:ARG:NE	2.54	0.41
1:F:938:TRP:HZ3	1:F:952:ARG:HH21	1.69	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:B:783:ALA:O	1:B:786:GLN:HG2	2.20	0.41
1:F:722:LEU:HD12	1:F:787:VAL:HG13	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:D:53:VAL:HG22	1:D:123:ALA:HB2	2.02	0.40
1:F:791:ARG:NE	1:F:793:ALA:HB2	2.36	0.40
1:A:21:ALA:O	1:A:25:LEU:HG	2.21	0.40
1:B:292:PRO:O	1:B:296:MET:HB2	2.21	0.40
1:A:210:ASN:ND2	1:A:210:ASN:O	2.55	0.40
1:F:34:LEU:HA	1:F:34:LEU:HD12	1.96	0.40
1:C:561:LEU:HB2	1:C:607:SER:O	2.21	0.40
1:A:893:LEU:HD22	1:A:1003:LEU:HD22	2.04	0.40
1:F:617:PRO:HB2	1:F:620:THR:HG22	2.03	0.40
1:C:826:ALA:O	1:C:830:ILE:HG12	2.21	0.40
1:E:203:THR:HG21	1:E:735:THR:HG21	2.04	0.40
1:C:871:PHE:HB2	1:C:888:LEU:HD21	2.03	0.40
1:C:137:ILE:HD13	1:C:286:LEU:HD13	2.03	0.40
1:A:736:GLY:O	1:A:758:PHE:HB2	2.22	0.40
1:F:859:LEU:HD21	1:F:914:ALA:HB1	2.03	0.40
1:E:436:ILE:HD13	1:E:436:ILE:HA	1.84	0.40
1:E:559:VAL:HG22	1:E:646:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:VAL:N	1:A:754:VAL:O	2.54	0.40
1:E:690:LEU:HD21	1:E:830:ILE:HD11	2.02	0.40
1:B:133:PRO:HG2	1:B:656:VAL:HG12	2.03	0.40
1:C:295:VAL:O	1:C:299:VAL:HG23	2.21	0.40
1:E:533:VAL:HA	1:E:536:MET:HE2	2.03	0.40
1:A:157:PHE:CE2	1:A:180:THR:HG22	2.56	0.40
1:A:608:HIS:CE1	1:A:610:GLU:HG3	2.57	0.40
1:A:547:LEU:HA	1:A:548:PRO:HD2	1.96	0.40
1:E:584:PHE:HA	1:E:585:PRO:HD3	1.82	0.40
1:C:913:SER:HB3	1:C:988:PRO:HB3	2.03	0.40
1:A:562:PRO:HD3	1:A:643:GLY:O	2.21	0.40
1:A:830:ILE:HD12	1:A:845:TRP:CZ2	2.57	0.40
1:F:138:TYR:CE2	1:F:319:PRO:HB3	2.56	0.40
1:B:203:THR:HG21	1:B:735:THR:HG21	2.02	0.40
1:D:544:ARG:HB2	1:D:820:SER:OG	2.21	0.40
1:D:276:ASN:ND2	1:D:279:THR:HB	2.36	0.40
1:E:187:PHE:HE2	1:E:756:ALA:HB1	1.86	0.40
1:C:565:ILE:HG22	1:C:566:SER:O	2.21	0.40
1:E:894:ALA:HB1	1:E:920:LEU:HG	2.03	0.40
1:C:546:PHE:CD2	1:C:851:ASN:HB3	2.57	0.40
1:D:166:GLN:HG2	1:E:74:MET:HE2	2.03	0.40
1:A:34:LEU:HA	1:A:34:LEU:HD12	1.92	0.40
1:B:36:LEU:HA	1:B:36:LEU:HD23	1.82	0.40
1:D:446:ALA:O	1:D:449:PRO:HD2	2.22	0.40
1:A:544:ARG:HB2	1:A:820:SER:OG	2.21	0.40
1:B:271:LEU:CD2	1:B:281:GLN:HB3	2.48	0.40
1:F:556:TRP:CZ2	1:F:610:GLU:HB3	2.57	0.40
1:D:456:ILE:HD11	1:D:546:PHE:CE1	2.56	0.40
1:A:703:GLN:HE21	1:A:800:THR:HG21	1.86	0.40
1:A:232:LEU:HD12	1:A:232:LEU:HA	1.93	0.40
1:D:703:GLN:HE21	1:D:800:THR:HG21	1.86	0.40
1:F:504:VAL:O	1:F:508:PRO:HD3	2.20	0.40
1:E:783:ALA:O	1:E:786:GLN:HG2	2.21	0.40
1:A:400:GLY:O	1:A:403:VAL:HG22	2.21	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%)	12	48
1	B	936/1045 (90%)	858 (92%)	76 (8%)	2 (0%)	52	88
1	C	943/1045 (90%)	850 (90%)	82 (9%)	11 (1%)	16	56
1	D	944/1045 (90%)	836 (89%)	93 (10%)	15 (2%)	12	48
1	E	936/1045 (90%)	860 (92%)	74 (8%)	2 (0%)	52	88
1	F	943/1045 (90%)	851 (90%)	81 (9%)	11 (1%)	16	56
All	All	5646/6270 (90%)	5092 (90%)	498 (9%)	56 (1%)	19	61

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%)	755 (96%)	32 (4%)	37	76
1	B	784/864 (91%)	746 (95%)	38 (5%)	31	71
1	C	789/864 (91%)	746 (95%)	43 (5%)	27	66
1	D	787/864 (91%)	756 (96%)	31 (4%)	39	77
1	E	784/864 (91%)	747 (95%)	37 (5%)	32	72
1	F	789/864 (91%)	747 (95%)	42 (5%)	28	67
All	All	4720/5184 (91%)	4497 (95%)	223 (5%)	32	72

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

Some 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	958/1045 (91%)	-0.37	24 (2%) 61 30	29, 77, 143, 215	0
1	B	954/1045 (91%)	-0.44	13 (1%) 78 51	27, 70, 135, 209	0
1	C	959/1045 (91%)	-0.39	21 (2%) 65 35	26, 71, 140, 241	0
1	D	958/1045 (91%)	-0.31	29 (3%) 54 25	29, 77, 142, 215	0
1	E	954/1045 (91%)	-0.44	15 (1%) 74 47	25, 70, 134, 209	0
1	F	959/1045 (91%)	-0.40	18 (1%) 70 41	26, 71, 139, 241	0
All	All	5742/6270 (91%)	-0.39	120 (2%) 67 36	25, 73, 140, 241	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	518	VAL	7.5
1	F	979	HIS	5.7
1	D	522	ARG	5.5
1	A	522	ARG	5.5
1	A	504	VAL	5.2
1	F	515	ASN	5.1
1	F	522	ARG	4.9
1	C	948	GLU	4.9
1	C	11	ASN	4.8
1	A	520	SER	4.8
1	F	505	TRP	4.5
1	D	504	VAL	4.5
1	D	208	GLU	4.3
1	D	979	HIS	4.3
1	A	100	GLY	4.1
1	E	454	GLN	4.0
1	E	11	ASN	3.9
1	E	518	VAL	3.9
1	D	523	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	832	LYS	3.8
1	F	502	ALA	3.7
1	A	521	THR	3.7
1	D	978	ALA	3.6
1	C	100	GLY	3.5
1	F	952	ARG	3.5
1	F	454	GLN	3.5
1	C	504	VAL	3.5
1	D	836	TYR	3.5
1	A	11	ASN	3.4
1	E	948	GLU	3.4
1	E	502	ALA	3.3
1	D	520	SER	3.3
1	C	952	ARG	3.3
1	D	505	TRP	3.2
1	E	522	ARG	3.2
1	A	781	HIS	3.1
1	D	629	GLN	3.1
1	A	979	HIS	3.1
1	A	258	GLY	3.1
1	D	508	PRO	3.1
1	C	454	GLN	3.0
1	B	454	GLN	3.0
1	C	71	ARG	3.0
1	A	1012	TYR	2.9
1	E	781	HIS	2.9
1	A	831	ASP	2.9
1	B	426	MET	2.9
1	B	12	ARG	2.9
1	B	522	ARG	2.9
1	D	777	ALA	2.8
1	F	622	THR	2.8
1	E	505	TRP	2.8
1	D	524	ALA	2.8
1	E	509	ARG	2.8
1	B	509	ARG	2.7
1	C	519	GLY	2.7
1	F	411	ARG	2.7
1	C	505	TRP	2.7
1	D	427	GLN	2.7
1	C	522	ARG	2.6
1	D	54	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	521	THR	2.6
1	F	55	GLY	2.6
1	C	838	ARG	2.6
1	A	502	ALA	2.5
1	D	502	ALA	2.5
1	C	979	HIS	2.5
1	F	518	VAL	2.5
1	A	523	THR	2.5
1	D	509	ARG	2.5
1	D	411	ARG	2.5
1	E	426	MET	2.5
1	A	840	HIS	2.5
1	A	208	GLU	2.5
1	A	196	ASN	2.5
1	A	505	TRP	2.5
1	E	521	THR	2.5
1	D	717	ALA	2.4
1	F	695	GLY	2.4
1	A	190	VAL	2.4
1	C	350	LEU	2.4
1	F	938	TRP	2.4
1	B	505	TRP	2.4
1	C	55	GLY	2.4
1	B	824	GLU	2.4
1	D	528	ALA	2.4
1	F	945	SER	2.3
1	E	978	ALA	2.3
1	D	526	GLY	2.3
1	B	15	ILE	2.3
1	C	904	LEU	2.3
1	D	11	ASN	2.3
1	C	945	SER	2.3
1	B	523	THR	2.3
1	D	512	SER	2.3
1	F	944	VAL	2.2
1	B	487	ALA	2.2
1	D	840	HIS	2.2
1	C	10	PHE	2.2
1	D	122	GLY	2.2
1	D	527	ILE	2.2
1	A	629	GLN	2.2
1	C	508	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	54	ASN	2.2
1	D	1014	LEU	2.2
1	A	516	ARG	2.2
1	C	509	ARG	2.1
1	B	10	PHE	2.1
1	F	937	ARG	2.1
1	C	54	ASN	2.1
1	E	100	GLY	2.1
1	F	380	PHE	2.1
1	A	339	MET	2.1
1	A	54	ASN	2.1
1	B	629	GLN	2.0
1	D	100	GLY	2.0
1	B	502	ALA	2.0
1	A	116	GLY	2.0
1	F	834	VAL	2.0
1	E	939	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	E	1101	1/1	0.88	0.09	-3.48	99,99,99,99	0
2	ZN	B	1101	1/1	0.96	0.04	-	108,108,108,108	0
2	ZN	D	1101	1/1	0.97	0.08	-	111,111,111,111	1
2	ZN	A	1101	1/1	0.96	0.08	-	112,112,112,112	0

## 6.5 Other polymers

There are no such residues in this entry.