



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 10:35 am GMT

PDB ID : 1PP6  
Title : VVA2 (STRIP CRYSTAL FORM)  
Authors : Lin, S.-C.; Lo, Y.-C.; Lin, J.-Y.; Liaw, Y.-C.  
Deposited on : 2003-06-16  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

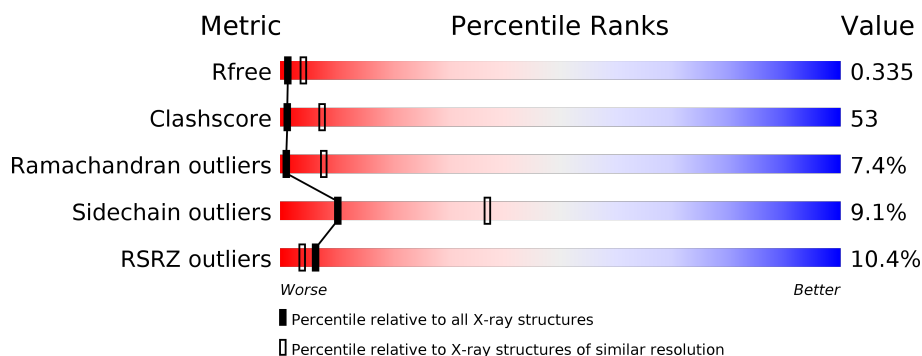
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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	199	<div> <div>0%</div> <div> <div>30%</div> <div>59%</div> <div>9%</div> </div> <div> <div>10%</div> <div>29%</div> <div>56%</div> <div>13%</div> </div> </div>
1	B	199	<div> <div>2%</div> <div> <div>32%</div> <div>56%</div> <div>9%</div> </div> <div> <div>10%</div> <div>29%</div> <div>56%</div> <div>13%</div> </div> </div>
1	C	199	<div> <div>3%</div> <div> <div>26%</div> <div>57%</div> <div>14%</div> </div> <div> <div>10%</div> <div>29%</div> <div>56%</div> <div>13%</div> </div> </div>
1	D	199	<div> <div>10%</div> <div> <div>29%</div> <div>56%</div> <div>13%</div> </div> <div> <div>10%</div> <div>29%</div> <div>56%</div> <div>13%</div> </div> </div>
1	E	199	<div> <div>35%</div> <div> <div>34%</div> <div>53%</div> <div>6%</div> </div> <div> <div>10%</div> <div>29%</div> <div>56%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7686 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 Volvatoxin A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1547	1004	241	301	1			
1	B	194	Total	C	N	O	S	0	0	0
			1547	1004	241	301	1			
1	C	194	Total	C	N	O	S	0	0	0
			1547	1004	241	301	1			
1	D	194	Total	C	N	O	S	0	0	0
			1547	1004	241	301	1			
1	E	186	Total	C	N	O	S	0	0	0
			1486	970	229	286	1			

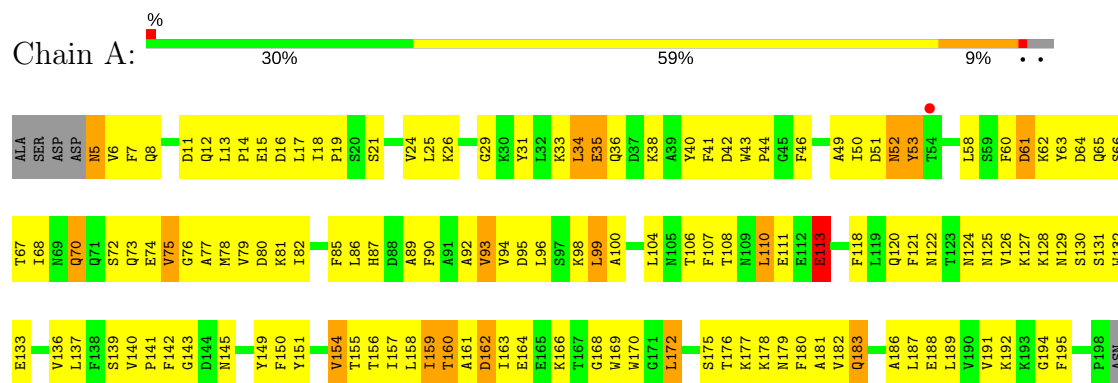
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	2	Total	O	0	0
			2	2		
2	C	3	Total	O	0	0
			3	3		
2	D	1	Total	O	0	0
			1	1		
2	E	4	Total	O	0	0
			4	4		

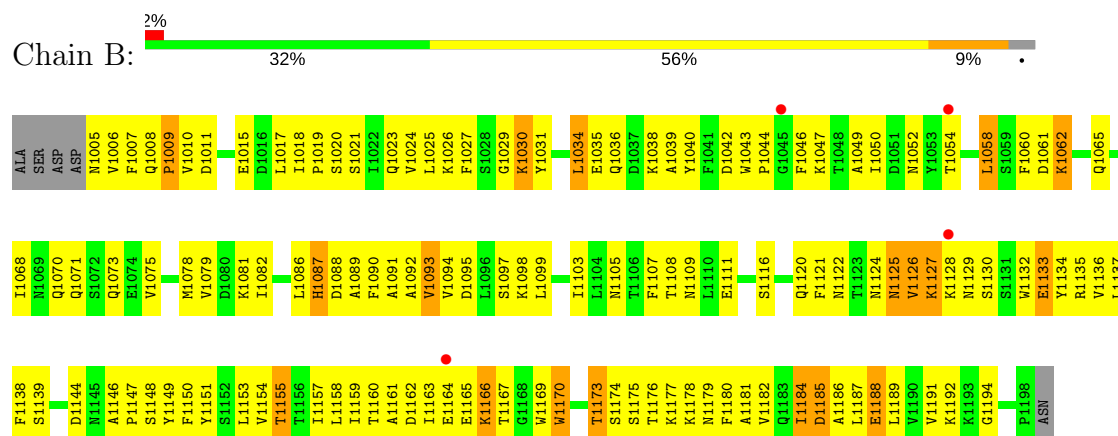
### 3 Residue-property plots

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

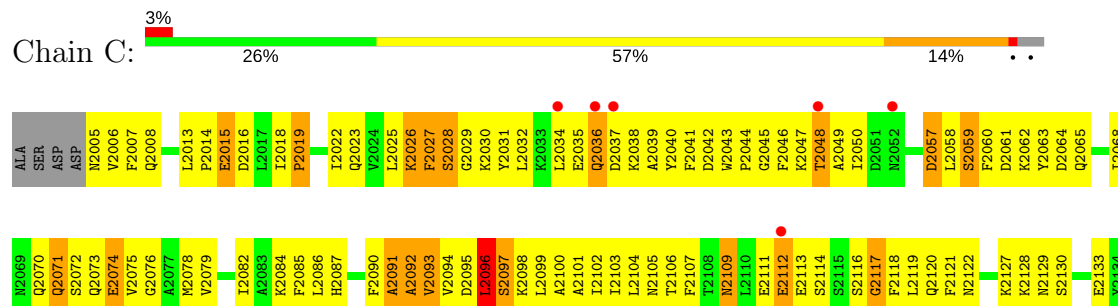
#### • Molecule 1: Volvatoxin A2



#### • Molecule 1: Volvatoxin A2

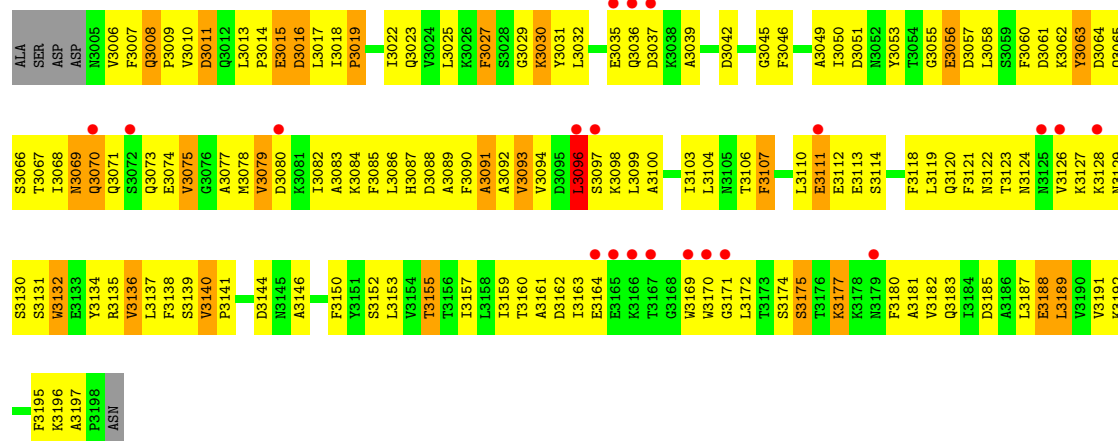


#### • Molecule 1: Volvatoxin A2

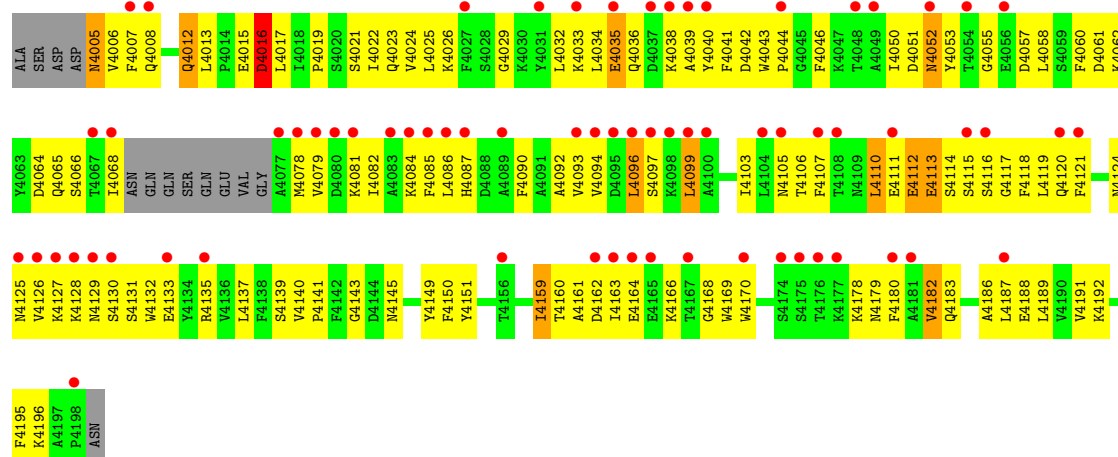




• Molecule 1: Volvatoxin A2



• Molecule 1: Volvatoxin A2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.67Å 80.68Å 107.85Å 90.00° 105.33° 90.00°	Depositor
Resolution (Å)	28.54 – 3.20 28.54 – 3.18	Depositor EDS
% Data completeness (in resolution range)	93.5 (28.54-3.20) 93.0 (28.54-3.18)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.83 (at 3.17Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.264 , 0.348 0.258 , 0.335	Depositor DCC
$R_{free}$ test set	1817 reflections (9.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 93.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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	0.55	0/1584	0.75	0/2150
1	B	0.54	0/1584	0.70	0/2150
1	C	0.54	0/1584	0.70	0/2150
1	D	0.48	0/1584	0.66	0/2150
1	E	0.51	0/1522	0.75	0/2065
All	All	0.53	0/7858	0.71	0/10665

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	3063	TYR	Sidechain

### 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	1547	0	1515	165	0
1	B	1547	0	1515	145	0
1	C	1547	0	1515	184	0
1	D	1547	0	1515	176	0
1	E	1486	0	1461	151	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	1	0
2	D	1	0	0	0	0
2	E	4	0	0	1	0
All	All	7686	0	7521	801	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 53.

All (801) 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:3013:LEU:HD22	1:D:3017:LEU:HD23	1.41	1.00
1:E:4006:VAL:HG11	1:E:4032:LEU:HD11	1.45	0.97
1:E:4006:VAL:HG23	1:E:4007:PHE:HD2	1.29	0.95
1:A:131:SER:HB3	1:A:160:THR:HG23	1.47	0.94
1:E:4106:THR:HG23	1:E:4113:GLU:HG2	1.47	0.94
1:E:4140:VAL:HB	1:E:4141:PRO:HD2	1.48	0.93
1:A:140:VAL:HB	1:A:141:PRO:HD2	1.51	0.92
1:D:3136:VAL:HG23	1:D:3155:THR:HG23	1.51	0.91
1:D:3122:ASN:HB3	1:D:3131:SER:HB2	1.53	0.91
1:E:4068:ILE:HB	1:E:4182:VAL:HG22	1.52	0.90
1:A:159:ILE:HA	1:A:182:VAL:HG12	1.50	0.90
1:D:3039:ALA:N	1:D:3120:GLN:HE21	1.70	0.89
1:D:3039:ALA:H	1:D:3120:GLN:HE21	0.92	0.88
1:D:3070:GLN:HA	1:D:3181:ALA:HB2	1.55	0.88
1:A:90:PHE:C	1:A:92:ALA:H	1.77	0.87
1:D:3039:ALA:H	1:D:3120:GLN:NE2	1.73	0.87
1:B:1061:ASP:HB3	1:B:1188:GLU:HB3	1.56	0.86
1:D:3057:ASP:OD1	1:D:3195:PHE:HA	1.74	0.85
1:D:3023:GLN:HG2	1:D:3196:LYS:HA	1.57	0.85
1:E:4131:SER:HB3	1:E:4160:THR:HG23	1.59	0.84
1:C:2070:GLN:HA	1:C:2180:PHE:O	1.77	0.84
1:E:4006:VAL:HG23	1:E:4007:PHE:CD2	2.13	0.84
1:E:4078:MET:CE	1:E:4182:VAL:HG11	2.08	0.84
1:C:2006:VAL:HG12	1:C:2135:ARG:HE	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2035:GLU:HG2	1:C:2036:GLN:H	1.44	0.81
1:B:1120:GLN:HB3	1:B:1133:GLU:HB3	1.63	0.80
1:D:3090:PHE:HB3	1:D:3188:GLU:OE2	1.82	0.80
1:C:2096:LEU:CD2	1:C:2097:SER:H	1.95	0.79
1:B:1132:TRP:O	1:B:1158:LEU:HD12	1.83	0.79
1:A:78:MET:HE3	1:A:182:VAL:HG11	1.65	0.78
1:C:2026:LYS:O	1:C:2028:SER:N	2.17	0.78
1:E:4078:MET:HE3	1:E:4182:VAL:HG11	1.64	0.78
1:B:1160:THR:HB	1:B:1181:ALA:HB3	1.63	0.78
1:D:3090:PHE:O	1:D:3092:ALA:N	2.17	0.77
1:E:4046:PHE:CZ	1:E:4050:ILE:HD11	2.20	0.77
1:D:3107:PHE:O	1:D:3110:LEU:HG	1.83	0.77
1:B:1157:ILE:HG12	1:B:1184:ILE:HG22	1.67	0.76
1:A:6:VAL:HG23	1:A:7:PHE:HD2	1.50	0.76
1:C:2035:GLU:HG2	1:C:2036:GLN:N	1.98	0.76
1:E:4120:GLN:HB3	1:E:4133:GLU:HB3	1.68	0.76
1:E:4086:LEU:HB3	1:E:4094:VAL:HG21	1.68	0.76
1:C:2032:LEU:HA	1:C:2042:ASP:H	1.50	0.76
1:E:4013:LEU:HD21	1:E:4021:SER:OG	1.86	0.76
1:E:4107:PHE:HA	1:E:4110:LEU:HD23	1.68	0.75
1:D:3042:ASP:OD1	1:D:3045:GLY:HA3	1.87	0.74
1:A:124:ASN:HD22	1:A:127:LYS:H	1.34	0.74
1:A:120:GLN:HB3	1:A:133:GLU:HB3	1.68	0.74
1:A:6:VAL:HG23	1:A:7:PHE:CD2	2.22	0.74
1:A:26:LYS:HE3	1:D:3061:ASP:O	1.87	0.74
1:C:2025:LEU:HD23	1:C:2137:LEU:HD12	1.67	0.74
1:E:4078:MET:HA	1:E:4081:LYS:HZ3	1.52	0.74
1:B:1007:PHE:O	1:B:1009:PRO:HD3	1.88	0.74
1:E:4132:TRP:HB2	1:E:4159:ILE:HG13	1.68	0.74
1:A:15:GLU:O	1:A:19:PRO:HD3	1.88	0.74
1:C:2013:LEU:HD11	1:C:2139:SER:HB3	1.70	0.73
1:C:2029:GLY:O	1:C:2032:LEU:HD22	1.88	0.73
1:B:1177:LYS:O	1:B:1178:LYS:HG3	1.87	0.73
1:E:4087:HIS:HD2	1:E:4096:LEU:H	1.37	0.73
1:C:2169:TRP:O	1:C:2172:LEU:HG	1.89	0.73
1:A:124:ASN:HD22	1:A:127:LYS:HB2	1.53	0.73
1:E:4050:ILE:HD13	1:E:4189:LEU:HD21	1.70	0.72
1:B:1073:GLN:HE21	1:B:1078:MET:HA	1.54	0.72
1:B:1173:THR:HG22	1:B:1176:THR:N	2.05	0.72
1:E:4006:VAL:HG21	1:E:4029:GLY:HA2	1.71	0.72
1:B:1006:VAL:HG21	1:B:1029:GLY:HA2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2130:SER:OG	1:C:2163:ILE:HB	1.88	0.72
1:C:2071:GLN:O	1:C:2179:ASN:HA	1.89	0.72
1:E:4078:MET:HA	1:E:4081:LYS:NZ	2.03	0.72
1:D:3159:ILE:HD13	1:D:3182:VAL:HB	1.72	0.72
1:A:124:ASN:ND2	1:A:127:LYS:H	1.88	0.72
1:E:4033:LYS:HG2	1:E:4040:TYR:O	1.90	0.72
1:D:3079:VAL:HG21	1:D:3104:LEU:HD13	1.71	0.72
1:B:1124:ASN:HB2	1:B:1129:ASN:OD1	1.89	0.71
1:D:3107:PHE:CZ	1:D:3159:ILE:HG13	2.25	0.71
1:C:2042:ASP:OD2	1:C:2045:GLY:HA3	1.91	0.71
1:C:2075:VAL:HB	1:C:2174:SER:O	1.90	0.71
1:B:1173:THR:HG23	1:B:1175:SER:H	1.55	0.71
1:D:3132:TRP:HE1	1:D:3169:TRP:HB2	1.56	0.71
1:A:121:PHE:HB2	1:A:132:TRP:CZ3	2.26	0.71
1:A:70:GLN:HB3	1:A:181:ALA:HB2	1.73	0.70
1:E:4005:ASN:ND2	1:E:4025:LEU:HD21	2.06	0.70
1:E:4034:LEU:O	1:E:4035:GLU:HB2	1.90	0.70
1:D:3075:VAL:O	1:D:3079:VAL:HG23	1.90	0.70
1:E:4132:TRP:HB2	1:E:4159:ILE:CG1	2.20	0.70
1:D:3132:TRP:HE1	1:D:3169:TRP:CB	2.05	0.70
1:C:2096:LEU:HD23	1:C:2097:SER:H	1.56	0.70
1:A:159:ILE:HG22	1:A:182:VAL:HG11	1.72	0.69
1:C:2007:PHE:CD1	1:C:2135:ARG:HB3	2.26	0.69
1:A:132:TRP:HB2	1:A:159:ILE:CG1	2.21	0.69
1:A:78:MET:CE	1:A:182:VAL:HG11	2.22	0.69
1:E:4005:ASN:HD21	1:E:4025:LEU:HD21	1.55	0.69
1:C:2074:GLU:OE1	1:C:2074:GLU:N	2.25	0.69
1:D:3153:LEU:CD2	1:D:3188:GLU:HB2	2.23	0.68
1:B:1173:THR:HG23	1:B:1174:SER:N	2.08	0.68
1:A:90:PHE:C	1:A:92:ALA:N	2.46	0.68
1:A:61:ASP:OD2	1:A:188:GLU:HG2	1.93	0.68
1:B:1159:ILE:HD12	1:B:1159:ILE:N	2.09	0.68
1:C:2128:LYS:NZ	1:D:3098:LYS:HZ2	1.92	0.68
1:B:1170:TRP:N	1:B:1170:TRP:HE3	1.93	0.67
1:B:1124:ASN:O	1:B:1126:VAL:N	2.24	0.67
1:C:2061:ASP:O	1:E:4026:LYS:HE3	1.94	0.67
1:A:43:TRP:CZ3	1:A:187:LEU:HB2	2.29	0.67
1:C:2050:ILE:HG21	1:C:2060:PHE:HB2	1.77	0.67
1:E:4061:ASP:OD2	1:E:4188:GLU:HG2	1.94	0.67
1:C:2142:PHE:HZ	1:E:4022:ILE:HD11	1.59	0.67
1:A:13:LEU:HD21	1:A:21:SER:OG	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2070:GLN:HE21	1:C:2179:ASN:HB3	1.58	0.67
1:E:4131:SER:CB	1:E:4160:THR:HA	2.25	0.67
1:A:36:GLN:O	1:A:38:LYS:HG3	1.95	0.67
1:A:11:ASP:HB2	1:A:13:LEU:HG	1.77	0.66
1:D:3135:ARG:HD2	1:D:3135:ARG:N	2.10	0.66
1:D:3030:LYS:O	1:D:3030:LYS:HG3	1.95	0.66
1:B:1006:VAL:CG2	1:B:1029:GLY:HA2	2.25	0.66
1:A:6:VAL:HG21	1:A:29:GLY:HA2	1.78	0.66
1:B:1173:THR:HG22	1:B:1176:THR:H	1.60	0.66
1:C:2070:GLN:NE2	1:C:2179:ASN:HB3	2.10	0.66
1:D:3077:ALA:O	1:D:3080:ASP:HB2	1.96	0.66
1:B:1146:ALA:HB1	1:B:1149:TYR:HB2	1.77	0.66
1:C:2006:VAL:HA	1:C:2117:GLY:O	1.95	0.66
1:B:1054:THR:O	1:B:1054:THR:HG23	1.96	0.66
1:C:2035:GLU:HG2	1:C:2036:GLN:HG2	1.78	0.65
1:A:13:LEU:HD12	1:A:13:LEU:O	1.97	0.65
1:C:2103:ILE:O	1:C:2103:ILE:HG22	1.94	0.65
1:E:4094:VAL:HG13	1:E:4099:LEU:HD22	1.78	0.65
1:E:4139:SER:HA	1:E:4151:TYR:O	1.95	0.65
1:C:2037:ASP:C	1:C:2038:LYS:HD2	2.16	0.65
1:D:3103:ILE:O	1:D:3103:ILE:HG22	1.95	0.65
1:A:50:ILE:HD13	1:A:189:LEU:HD21	1.79	0.64
1:B:1087:HIS:HD2	1:B:1095:ASP:HA	1.62	0.64
1:D:3023:GLN:HG3	1:D:3197:ALA:H	1.62	0.64
1:D:3124:ASN:HB3	1:D:3127:LYS:HG2	1.80	0.64
1:B:1162:ASP:OD2	1:B:1179:ASN:HB2	1.98	0.64
1:E:4062:LYS:NZ	1:E:4064:ASP:HB2	2.13	0.64
1:A:24:VAL:HG21	1:A:191:VAL:HG21	1.78	0.64
1:A:132:TRP:HB2	1:A:159:ILE:HG13	1.80	0.64
1:B:1163:ILE:HD11	1:B:1178:LYS:HD3	1.80	0.64
1:D:3121:PHE:HB2	1:D:3132:TRP:CH2	2.33	0.64
1:D:3137:LEU:HA	1:D:3153:LEU:O	1.98	0.63
1:C:2090:PHE:O	1:C:2091:ALA:C	2.36	0.63
1:D:3153:LEU:HD22	1:D:3188:GLU:HB2	1.81	0.63
1:A:61:ASP:O	1:A:62:LYS:HB2	1.98	0.63
1:A:25:LEU:HD13	1:A:137:LEU:HD23	1.81	0.63
1:A:42:ASP:OD1	1:A:44:PRO:HD2	1.98	0.63
1:B:1062:LYS:HE3	1:B:1188:GLU:HG3	1.79	0.63
1:C:2128:LYS:HZ3	1:D:3098:LYS:HZ2	1.44	0.63
1:D:3027:PHE:HD1	1:D:3027:PHE:O	1.82	0.63
1:D:3075:VAL:HG22	1:D:3180:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:LYS:O	1:B:1178:LYS:CG	2.46	0.63
1:C:2035:GLU:HB3	1:C:2038:LYS:O	1.99	0.63
1:C:2090:PHE:O	1:C:2092:ALA:N	2.32	0.62
1:C:2058:LEU:HD12	1:C:2195:PHE:CE1	2.34	0.62
1:B:1090:PHE:O	1:B:1093:VAL:N	2.32	0.62
1:B:1075:VAL:HG21	1:B:1173:THR:O	1.99	0.62
1:E:4078:MET:HE1	1:E:4182:VAL:HG11	1.79	0.62
1:C:2093:VAL:HG13	1:C:2094:VAL:HG23	1.82	0.62
1:B:1139:SER:HA	1:B:1151:TYR:O	2.00	0.62
1:C:2061:ASP:OD1	1:E:4026:LYS:HE2	1.98	0.62
1:E:4149:TYR:CZ	1:E:4192:LYS:HD3	2.35	0.62
1:A:159:ILE:HG22	1:A:182:VAL:CG1	2.29	0.62
1:D:3098:LYS:HZ2	1:D:3098:LYS:HB2	1.65	0.62
1:B:1111:GLU:HB3	1:D:3069:ASN:CG	2.21	0.61
1:D:3015:GLU:O	1:D:3017:LEU:N	2.33	0.61
1:E:4149:TYR:CE1	1:E:4192:LYS:HB2	2.35	0.61
1:D:3074:GLU:O	1:D:3077:ALA:HB3	2.00	0.61
1:A:68:ILE:HB	1:A:182:VAL:HG22	1.80	0.61
1:C:2039:ALA:O	1:C:2120:GLN:HG2	2.00	0.61
1:C:2013:LEU:HB3	1:C:2014:PRO:HD2	1.82	0.61
1:C:2032:LEU:HB2	1:C:2040:TYR:O	2.00	0.61
1:E:4006:VAL:CG2	1:E:4029:GLY:HA2	2.30	0.61
1:E:4162:ASP:OD1	1:E:4179:ASN:HB2	2.01	0.61
1:A:124:ASN:ND2	1:A:127:LYS:HB2	2.16	0.61
1:D:3015:GLU:HG3	1:D:3016:ASP:N	2.16	0.61
1:E:4093:VAL:HG13	1:E:4140:VAL:HG22	1.82	0.61
1:C:2121:PHE:CE2	1:C:2166:LYS:HB3	2.36	0.61
1:B:1184:ILE:HD13	1:B:1184:ILE:H	1.66	0.61
1:D:3009:PRO:HB3	1:D:3025:LEU:HD22	1.82	0.61
1:C:2091:ALA:C	1:C:2093:VAL:H	2.04	0.60
1:E:4006:VAL:CG1	1:E:4032:LEU:HD11	2.27	0.60
1:D:3098:LYS:NZ	1:D:3098:LYS:HB2	2.17	0.60
1:D:3007:PHE:CD1	1:D:3135:ARG:HB3	2.35	0.60
1:B:1184:ILE:N	1:B:1184:ILE:HD13	2.16	0.60
1:D:3121:PHE:HB2	1:D:3132:TRP:CZ3	2.36	0.60
1:B:1090:PHE:CD1	1:B:1188:GLU:HG2	2.36	0.60
1:E:4050:ILE:CG2	1:E:4060:PHE:HB2	2.32	0.60
1:B:1159:ILE:HD12	1:B:1159:ILE:H	1.66	0.60
1:C:2121:PHE:CE1	1:C:2130:SER:HB2	2.36	0.60
1:C:2121:PHE:CD2	1:C:2166:LYS:HB3	2.36	0.60
1:E:4090:PHE:C	1:E:4092:ALA:H	2.03	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4140:VAL:HB	1:E:4141:PRO:CD	2.28	0.60
1:D:3015:GLU:HG3	1:D:3016:ASP:H	1.67	0.60
1:E:4107:PHE:CE1	1:E:4159:ILE:HD13	2.37	0.59
1:C:2079:VAL:HG21	1:C:2104:LEU:HD13	1.83	0.59
1:A:62:LYS:NZ	1:A:63:TYR:O	2.34	0.59
1:E:4017:LEU:HD13	1:E:4150:PHE:HB3	1.83	0.59
1:B:1132:TRP:O	1:B:1158:LEU:HA	2.03	0.59
1:C:2008:GLN:HE22	1:C:2102:ILE:CG2	2.15	0.59
1:D:3087:HIS:HD2	1:D:3096:LEU:HB2	1.67	0.59
1:B:1090:PHE:C	1:B:1092:ALA:H	2.04	0.58
1:E:4023:GLN:HG3	1:E:4195:PHE:O	2.03	0.58
1:A:177:LYS:O	1:A:178:LYS:HD2	2.04	0.58
1:A:178:LYS:HB2	1:A:180:PHE:CZ	2.37	0.58
1:B:1154:VAL:O	1:B:1186:ALA:HA	2.04	0.58
1:C:2102:ILE:N	1:C:2102:ILE:HD12	2.18	0.58
1:A:96:LEU:O	1:A:99:LEU:HD21	2.02	0.58
1:B:1090:PHE:C	1:B:1092:ALA:N	2.55	0.58
1:B:1105:ASN:HD21	1:D:3183:GLN:HE22	1.49	0.58
1:B:1090:PHE:HD1	1:B:1188:GLU:CG	2.16	0.58
1:C:2008:GLN:HE22	1:C:2102:ILE:HG21	1.69	0.58
1:D:3015:GLU:C	1:D:3017:LEU:H	2.06	0.58
1:A:99:LEU:HG	1:A:100:ALA:N	2.19	0.58
1:B:1011:ASP:O	1:B:1011:ASP:OD2	2.21	0.58
1:A:124:ASN:HD22	1:A:127:LYS:N	1.99	0.58
1:A:124:ASN:HD22	1:A:127:LYS:CB	2.15	0.58
1:C:2078:MET:O	1:C:2082:ILE:HG13	2.04	0.58
1:B:1138:PHE:O	1:B:1153:LEU:N	2.34	0.58
1:C:2090:PHE:C	1:C:2092:ALA:N	2.50	0.58
1:C:2145:ASN:O	1:C:2146:ALA:HB2	2.03	0.58
1:D:3027:PHE:O	1:D:3030:LYS:HG2	2.04	0.58
1:D:3039:ALA:O	1:D:3120:GLN:HG2	2.04	0.58
1:B:1006:VAL:HG23	1:B:1007:PHE:CD2	2.39	0.58
1:D:3094:VAL:CG1	1:D:3099:LEU:HD22	2.34	0.58
1:B:1126:VAL:HG12	1:B:1127:LYS:N	2.19	0.57
1:B:1093:VAL:HG22	1:B:1151:TYR:CG	2.40	0.57
1:B:1170:TRP:CE3	1:B:1170:TRP:N	2.72	0.57
1:B:1090:PHE:O	1:B:1092:ALA:N	2.38	0.57
1:C:2013:LEU:HD23	1:C:2140:VAL:C	2.24	0.57
1:D:3062:LYS:HG2	1:D:3063:TYR:N	2.18	0.57
1:D:3121:PHE:CE1	1:D:3130:SER:HB3	2.39	0.57
1:E:4113:GLU:HB3	1:E:4119:LEU:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLN:HA	1:A:180:PHE:O	2.05	0.57
1:A:75:VAL:O	1:A:77:ALA:N	2.37	0.57
1:B:1127:LYS:HB3	1:B:1129:ASN:ND2	2.19	0.57
1:B:1157:ILE:HG12	1:B:1184:ILE:CG2	2.35	0.57
1:C:2035:GLU:CG	1:C:2036:GLN:H	2.14	0.57
1:C:2178:LYS:HB2	1:C:2180:PHE:CE2	2.40	0.57
1:C:2128:LYS:NZ	1:D:3098:LYS:NZ	2.52	0.57
1:E:4143:GLY:C	1:E:4145:ASN:H	2.07	0.57
1:C:2043:TRP:HB2	1:C:2044:PRO:HD3	1.87	0.57
1:D:3093:VAL:HG11	1:D:3153:LEU:HD23	1.87	0.57
1:E:4066:SER:HB2	1:E:4085:PHE:CE1	2.40	0.57
1:C:2090:PHE:HB3	1:C:2093:VAL:HG12	1.87	0.56
1:E:4068:ILE:HD13	1:E:4081:LYS:HD2	1.86	0.56
1:D:3073:GLN:HG2	1:D:3180:PHE:HB2	1.87	0.56
1:B:1136:VAL:HG13	1:B:1136:VAL:O	2.06	0.56
1:C:2013:LEU:HG	1:C:2139:SER:O	2.05	0.56
1:A:6:VAL:CG2	1:A:29:GLY:HA2	2.36	0.56
1:E:4121:PHE:HB2	1:E:4132:TRP:CZ3	2.40	0.56
1:A:161:ALA:HA	1:A:179:ASN:O	2.05	0.56
1:B:1090:PHE:HD1	1:B:1188:GLU:HG2	1.70	0.56
1:A:18:ILE:O	1:A:21:SER:HB2	2.05	0.56
1:A:149:TYR:CE1	1:A:192:LYS:HB2	2.41	0.56
1:B:1133:GLU:HG2	1:B:1135:ARG:NH1	2.20	0.56
1:C:2006:VAL:HG21	1:C:2029:GLY:CA	2.35	0.56
1:A:74:GLU:O	1:A:77:ALA:HB3	2.06	0.56
1:C:2006:VAL:O	1:C:2118:PHE:HA	2.05	0.56
1:C:2187:LEU:HD21	1:C:2189:LEU:HD21	1.88	0.56
1:D:3163:ILE:HD12	1:D:3169:TRP:CE2	2.41	0.56
1:E:4025:LEU:HD13	1:E:4137:LEU:HD23	1.87	0.56
1:A:78:MET:HE1	1:A:159:ILE:HG22	1.86	0.56
1:D:3094:VAL:HG11	1:D:3099:LEU:HD22	1.87	0.56
1:B:1035:GLU:O	1:B:1035:GLU:HG3	2.06	0.55
1:C:2073:GLN:O	1:C:2177:LYS:HA	2.06	0.55
1:B:1065:GLN:HG3	1:B:1185:ASP:OD2	2.05	0.55
1:B:1173:THR:HG23	1:B:1175:SER:N	2.20	0.55
1:C:2027:PHE:CG	1:C:2027:PHE:O	2.58	0.55
1:D:3078:MET:C	1:D:3080:ASP:H	2.10	0.55
1:D:3177:LYS:HB2	1:D:3177:LYS:NZ	2.21	0.55
1:E:4012:GLN:NE2	1:E:4141:PRO:HD2	2.20	0.55
1:A:82:ILE:HG21	1:A:157:ILE:HD11	1.86	0.55
1:A:163:ILE:HD11	1:A:178:LYS:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HG3	1:A:164:GLU:OE1	2.07	0.55
1:C:2023:GLN:O	1:C:2026:LYS:N	2.40	0.55
1:D:3009:PRO:HB3	1:D:3025:LEU:CD2	2.37	0.55
1:E:4124:ASN:HD22	1:E:4127:LYS:H	1.55	0.55
1:C:2008:GLN:NE2	1:C:2102:ILE:HG21	2.21	0.55
1:A:25:LEU:CD1	1:A:137:LEU:HD23	2.37	0.55
1:B:1062:LYS:HD2	1:B:1089:ALA:O	2.07	0.55
1:B:1018:ILE:HB	1:B:1019:PRO:HD3	1.89	0.55
1:B:1027:PHE:HZ	1:B:1049:ALA:HB1	1.72	0.55
1:D:3018:ILE:HB	1:D:3019:PRO:HD3	1.90	0.55
1:E:4114:SER:O	1:E:4116:SER:N	2.40	0.55
1:B:1007:PHE:CD1	1:B:1135:ARG:HB3	2.42	0.54
1:C:2035:GLU:CG	1:C:2036:GLN:N	2.70	0.54
1:D:3062:LYS:HE2	1:D:3089:ALA:O	2.08	0.54
1:E:4125:ASN:O	1:E:4128:LYS:HD2	2.06	0.54
1:B:1046:PHE:O	1:B:1047:LYS:C	2.46	0.54
1:E:4050:ILE:HG21	1:E:4060:PHE:HB2	1.90	0.54
1:E:4113:GLU:HB3	1:E:4119:LEU:HD12	1.87	0.54
1:A:8:GLN:NE2	1:A:118:PHE:CZ	2.75	0.54
1:C:2192:LYS:HG2	1:C:2193:LYS:N	2.22	0.54
1:D:3025:LEU:O	1:D:3025:LEU:HD12	2.08	0.54
1:D:3090:PHE:C	1:D:3092:ALA:N	2.57	0.54
1:A:78:MET:HE3	1:A:182:VAL:CG1	2.37	0.54
1:B:1075:VAL:O	1:B:1078:MET:HB3	2.07	0.54
1:E:4013:LEU:HD13	1:E:4017:LEU:HB3	1.89	0.54
1:C:2038:LYS:HG2	1:C:2122:ASN:HD22	1.71	0.54
1:B:1137:LEU:HD13	1:B:1154:VAL:HG22	1.89	0.54
1:C:2091:ALA:O	1:C:2093:VAL:N	2.37	0.54
1:E:4166:LYS:C	1:E:4168:GLY:N	2.60	0.54
1:A:107:PHE:CE1	1:A:159:ILE:HD13	2.43	0.53
1:A:149:TYR:CZ	1:A:192:LYS:HD3	2.43	0.53
1:B:1126:VAL:C	1:B:1128:LYS:H	2.12	0.53
1:C:2178:LYS:O	1:C:2180:PHE:HD2	1.90	0.53
1:C:2155:THR:HG23	1:C:2186:ALA:HB2	1.90	0.53
1:C:2068:ILE:HB	1:C:2182:VAL:HG13	1.90	0.53
1:A:74:GLU:HB3	1:A:177:LYS:HG2	1.90	0.53
1:D:3070:GLN:CA	1:D:3181:ALA:HB2	2.35	0.53
1:C:2064:ASP:OD2	1:C:2065:GLN:N	2.42	0.53
1:E:4006:VAL:HA	1:E:4117:GLY:O	2.07	0.53
1:E:4013:LEU:HD13	1:E:4017:LEU:CB	2.39	0.53
1:E:4081:LYS:HB2	1:E:4081:LYS:NZ	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1031:TYR:O	1:B:1042:ASP:HB3	2.08	0.53
1:E:4166:LYS:C	1:E:4168:GLY:H	2.10	0.53
1:A:58:LEU:HD21	1:A:189:LEU:HD13	1.90	0.53
1:B:1079:VAL:HG13	1:B:1103:ILE:CG2	2.38	0.53
1:D:3008:GLN:O	1:D:3010:VAL:HG23	2.08	0.53
1:B:1093:VAL:HG21	1:B:1188:GLU:OE2	2.08	0.53
1:C:2173:THR:O	1:C:2174:SER:C	2.47	0.53
1:A:78:MET:O	1:A:82:ILE:HG13	2.09	0.53
1:B:1073:GLN:HE21	1:B:1078:MET:CA	2.21	0.53
1:C:2099:LEU:C	1:C:2101:ALA:H	2.12	0.53
1:D:3007:PHE:O	1:D:3009:PRO:HD3	2.09	0.53
1:B:1073:GLN:NE2	1:B:1078:MET:HA	2.21	0.53
1:C:2121:PHE:HE1	1:C:2130:SER:HB2	1.74	0.53
1:E:4143:GLY:C	1:E:4145:ASN:N	2.63	0.53
1:C:2163:ILE:HG21	1:C:2169:TRP:CD1	2.44	0.52
1:B:1120:GLN:O	1:B:1132:TRP:HA	2.10	0.52
1:A:64:ASP:OD1	1:A:65:GLN:N	2.42	0.52
1:B:1040:TYR:OH	1:B:1122:ASN:HB2	2.09	0.52
1:E:4126:VAL:C	1:E:4128:LYS:H	2.13	0.52
1:D:3107:PHE:HA	1:D:3110:LEU:HG	1.92	0.52
1:E:4042:ASP:OD1	1:E:4044:PRO:HD2	2.09	0.52
1:A:63:TYR:CG	1:A:64:ASP:N	2.78	0.52
1:C:2006:VAL:HG21	1:C:2029:GLY:HA3	1.92	0.52
1:A:31:TYR:OH	1:A:49:ALA:HB1	2.10	0.52
1:D:3074:GLU:HB3	1:D:3077:ALA:HB3	1.90	0.52
1:A:161:ALA:HB2	1:A:180:PHE:CD1	2.44	0.52
1:E:4163:ILE:HD11	1:E:4178:LYS:HG2	1.91	0.52
1:B:1146:ALA:CB	1:B:1149:TYR:HB2	2.40	0.52
1:D:3087:HIS:CD2	1:D:3096:LEU:HB2	2.45	0.52
1:D:3135:ARG:C	1:D:3136:VAL:HG22	2.30	0.52
1:B:1098:LYS:HD3	1:B:1098:LYS:O	2.10	0.51
1:D:3083:ALA:HB1	1:D:3099:LEU:HD23	1.92	0.51
1:A:131:SER:HA	1:A:159:ILE:O	2.09	0.51
1:E:4131:SER:HB3	1:E:4160:THR:HA	1.92	0.51
1:A:50:ILE:HG21	1:A:60:PHE:HB2	1.92	0.51
1:C:2087:HIS:O	1:C:2091:ALA:N	2.43	0.51
1:D:3124:ASN:ND2	1:D:3126:VAL:HB	2.25	0.51
1:A:104:LEU:HD23	1:A:108:THR:HG23	1.93	0.51
1:C:2071:GLN:NE2	1:C:2073:GLN:NE2	2.59	0.51
1:A:14:PRO:HG2	1:A:17:LEU:HD12	1.92	0.51
1:C:2006:VAL:HG13	1:C:2135:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2087:HIS:HA	1:C:2094:VAL:HB	1.93	0.51
1:E:4150:PHE:CZ	1:E:4191:VAL:HB	2.46	0.51
1:B:1136:VAL:O	1:B:1155:THR:HG23	2.10	0.51
1:E:4187:LEU:C	1:E:4187:LEU:HD23	2.31	0.51
1:B:1015:GLU:O	1:B:1019:PRO:HD3	2.10	0.51
1:B:1011:ASP:C	1:B:1011:ASP:OD2	2.50	0.51
1:C:2075:VAL:O	1:C:2079:VAL:HG23	2.11	0.51
1:D:3074:GLU:HB3	1:D:3077:ALA:CB	2.40	0.51
1:E:4129:ASN:C	1:E:4129:ASN:OD1	2.49	0.51
1:C:2038:LYS:N	1:C:2038:LYS:HD2	2.26	0.51
1:C:2164:GLU:HA	1:C:2164:GLU:OE1	2.11	0.51
1:D:3130:SER:HB2	1:D:3169:TRP:HE1	1.76	0.51
1:C:2071:GLN:HE22	1:C:2073:GLN:NE2	2.08	0.50
1:C:2099:LEU:O	1:C:2101:ALA:N	2.44	0.50
1:B:1087:HIS:CD2	1:B:1095:ASP:HA	2.43	0.50
1:C:2106:THR:HA	1:C:2113:GLU:OE1	2.11	0.50
1:E:4131:SER:HA	1:E:4159:ILE:O	2.11	0.50
1:C:2032:LEU:HD23	1:C:2032:LEU:H	1.75	0.50
1:A:133:GLU:OE2	1:A:133:GLU:HA	2.12	0.50
1:A:162:ASP:OD1	1:A:179:ASN:HB2	2.11	0.50
1:C:2058:LEU:HD23	1:C:2059:SER:N	2.27	0.50
1:C:2005:ASN:O	1:C:2117:GLY:C	2.49	0.50
2:C:5002:HOH:O	1:E:4016:ASP:HB3	2.11	0.50
1:E:4041:PHE:HE1	1:E:4043:TRP:CD2	2.29	0.50
1:B:1109:ASN:OD1	1:D:3067:THR:HG21	2.10	0.50
1:D:3071:GLN:O	1:D:3180:PHE:N	2.45	0.50
1:E:4106:THR:CG2	1:E:4113:GLU:HG2	2.31	0.50
1:B:1050:ILE:HG21	1:B:1060:PHE:HB2	1.94	0.50
1:B:1187:LEU:HD23	1:B:1188:GLU:O	2.12	0.50
1:D:3060:PHE:HE1	1:D:3187:LEU:HG	1.76	0.50
1:A:31:TYR:OH	1:A:49:ALA:CB	2.60	0.50
1:C:2074:GLU:CD	1:C:2074:GLU:N	2.64	0.50
1:E:4178:LYS:CB	1:E:4180:PHE:CZ	2.95	0.50
1:C:2032:LEU:HD21	1:C:2034:LEU:HD11	1.93	0.50
1:C:2093:VAL:HG23	1:C:2140:VAL:HG22	1.93	0.50
1:D:3011:ASP:HB3	1:D:3139:SER:HB2	1.94	0.50
1:E:4140:VAL:CB	1:E:4141:PRO:CD	2.89	0.50
1:D:3015:GLU:CG	1:D:3016:ASP:H	2.24	0.50
1:D:3079:VAL:HA	1:D:3082:ILE:CG2	2.42	0.50
1:D:3032:LEU:CD1	1:D:3135:ARG:HH12	2.25	0.50
1:E:4078:MET:O	1:E:4082:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4163:ILE:HG21	1:E:4169:TRP:CD1	2.46	0.49
1:A:166:LYS:C	1:A:168:GLY:H	2.15	0.49
1:A:187:LEU:C	1:A:187:LEU:HD23	2.32	0.49
1:C:2090:PHE:CD1	1:C:2188:GLU:HB2	2.47	0.49
1:E:4112:GLU:O	1:E:4113:GLU:C	2.51	0.49
1:D:3018:ILE:N	1:D:3019:PRO:CD	2.75	0.49
1:D:3136:VAL:CG2	1:D:3155:THR:HG23	2.32	0.49
1:B:1127:LYS:HG3	1:B:1127:LYS:O	2.12	0.49
1:B:1163:ILE:HD11	1:B:1178:LYS:CD	2.42	0.49
1:C:2061:ASP:OD2	1:E:4022:ILE:HG21	2.12	0.49
1:B:1071:GLN:O	1:B:1179:ASN:HA	2.13	0.49
1:B:1165:GLU:C	1:B:1167:THR:H	2.16	0.49
1:C:2099:LEU:C	1:C:2101:ALA:N	2.66	0.49
1:B:1161:ALA:C	1:B:1163:ILE:H	2.15	0.49
1:D:3130:SER:O	1:D:3160:THR:HA	2.11	0.49
1:E:4041:PHE:HZ	1:E:4046:PHE:CD2	2.30	0.49
1:A:50:ILE:CG2	1:A:60:PHE:HB2	2.43	0.49
1:B:1173:THR:CG2	1:B:1174:SER:N	2.72	0.49
1:A:96:LEU:O	1:A:99:LEU:CD2	2.60	0.49
1:E:4023:GLN:HG3	1:E:4196:LYS:HA	1.94	0.49
1:B:1017:LEU:HD11	1:B:1147:PRO:O	2.13	0.49
1:B:1073:GLN:HE21	1:B:1078:MET:CB	2.26	0.49
1:D:3014:PRO:O	1:D:3015:GLU:C	2.51	0.49
1:D:3169:TRP:HA	1:D:3172:LEU:HD11	1.94	0.49
1:B:1075:VAL:HG23	1:B:1176:THR:O	2.13	0.49
1:E:4094:VAL:HG13	1:E:4099:LEU:HD13	1.94	0.49
1:B:1030:LYS:O	1:B:1031:TYR:CD2	2.66	0.48
1:E:4132:TRP:HB2	1:E:4159:ILE:CD1	2.42	0.48
1:A:31:TYR:HD2	1:A:46:PHE:HD1	1.61	0.48
1:C:2073:GLN:O	1:C:2177:LYS:HG3	2.12	0.48
1:E:4046:PHE:CE2	1:E:4050:ILE:HD11	2.47	0.48
1:E:4130:SER:HG	1:E:4169:TRP:HE1	1.60	0.48
1:A:66:SER:HB2	1:A:85:PHE:CE1	2.48	0.48
1:C:2023:GLN:OE1	1:C:2026:LYS:HD2	2.12	0.48
1:C:2062:LYS:HG2	1:C:2063:TYR:N	2.26	0.48
1:C:2137:LEU:O	1:C:2137:LEU:HD13	2.13	0.48
1:A:140:VAL:CB	1:A:141:PRO:HD2	2.30	0.48
1:A:178:LYS:CB	1:A:180:PHE:CZ	2.96	0.48
1:B:1036:GLN:C	1:B:1038:LYS:H	2.15	0.48
1:B:1097:SER:C	1:B:1099:LEU:N	2.64	0.48
1:C:2032:LEU:HA	1:C:2042:ASP:N	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3015:GLU:HA	1:D:3018:ILE:HG12	1.94	0.48
1:A:72:SER:HA	1:A:178:LYS:O	2.14	0.48
1:C:2094:VAL:HG13	1:C:2099:LEU:HD22	1.94	0.48
1:C:2149:TYR:CE1	1:C:2192:LYS:HB2	2.49	0.48
1:C:2167:THR:HG23	1:C:2170:TRP:CD1	2.48	0.48
1:D:3079:VAL:HA	1:D:3082:ILE:HG22	1.94	0.48
1:D:3150:PHE:CZ	1:D:3191:VAL:CG1	2.97	0.48
1:D:3172:LEU:HD12	1:D:3172:LEU:N	2.29	0.48
1:E:4126:VAL:HG23	1:E:4127:LYS:N	2.28	0.48
1:B:1043:TRP:O	1:B:1047:LYS:HG2	2.14	0.48
1:B:1079:VAL:HG13	1:B:1103:ILE:HG22	1.94	0.48
1:C:2113:GLU:O	1:C:2119:LEU:HD12	2.13	0.48
1:D:3015:GLU:CG	1:D:3016:ASP:N	2.76	0.48
1:E:4124:ASN:ND2	1:E:4127:LYS:HG3	2.29	0.48
1:A:139:SER:HA	1:A:151:TYR:O	2.13	0.48
1:A:166:LYS:C	1:A:168:GLY:N	2.66	0.48
1:A:150:PHE:CZ	1:A:191:VAL:HB	2.49	0.48
1:B:1166:LYS:HG2	1:B:1166:LYS:O	2.13	0.48
1:C:2041:PHE:HE1	1:C:2043:TRP:CE3	2.32	0.48
1:C:2092:ALA:O	1:C:2093:VAL:HB	2.12	0.48
1:D:3090:PHE:O	1:D:3091:ALA:C	2.51	0.48
1:E:4057:ASP:OD1	1:E:4057:ASP:N	2.41	0.48
1:E:4178:LYS:HB2	1:E:4180:PHE:CZ	2.48	0.48
1:D:3027:PHE:HD2	1:D:3195:PHE:HZ	1.61	0.48
1:A:132:TRP:HB2	1:A:159:ILE:HD11	1.95	0.48
1:B:1075:VAL:O	1:B:1079:VAL:HG23	2.14	0.48
1:D:3067:THR:O	1:D:3068:ILE:HD13	2.14	0.48
1:A:58:LEU:HB2	1:A:195:PHE:CD1	2.48	0.47
1:A:46:PHE:CZ	1:A:50:ILE:HD11	2.49	0.47
1:A:75:VAL:C	1:A:77:ALA:H	2.18	0.47
1:B:1009:PRO:HG3	1:B:1025:LEU:HD22	1.95	0.47
1:C:2133:GLU:OE2	1:C:2135:ARG:HG3	2.14	0.47
1:D:3027:PHE:C	1:D:3027:PHE:HD1	2.17	0.47
1:E:4090:PHE:C	1:E:4092:ALA:N	2.67	0.47
1:B:1126:VAL:O	1:B:1128:LYS:N	2.48	0.47
1:C:2093:VAL:HG22	1:C:2093:VAL:O	2.13	0.47
1:B:1043:TRP:CZ3	1:B:1187:LEU:HB2	2.49	0.47
1:C:2096:LEU:HD23	1:C:2097:SER:N	2.24	0.47
1:C:2137:LEU:C	1:C:2137:LEU:HD22	2.33	0.47
1:D:3013:LEU:HD11	1:D:3139:SER:HB3	1.96	0.47
1:C:2038:LYS:HG3	1:C:2120:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2163:ILE:HG21	1:C:2169:TRP:NE1	2.29	0.47
1:A:132:TRP:HB2	1:A:159:ILE:CD1	2.45	0.47
1:C:2014:PRO:O	1:C:2015:GLU:C	2.53	0.47
1:C:2058:LEU:HD23	1:C:2059:SER:H	1.78	0.47
1:D:3090:PHE:O	1:D:3093:VAL:N	2.47	0.47
1:E:4046:PHE:CG	1:E:4046:PHE:O	2.67	0.47
1:E:4132:TRP:HB2	1:E:4159:ILE:HD11	1.97	0.47
1:E:4081:LYS:O	1:E:4084:LYS:HB3	2.14	0.47
1:B:1163:ILE:HD11	1:B:1178:LYS:HE3	1.97	0.47
1:C:2018:ILE:O	1:C:2019:PRO:C	2.49	0.47
1:C:2047:LYS:O	1:C:2049:ALA:N	2.48	0.47
1:A:33:LYS:O	1:A:34:LEU:C	2.53	0.47
1:A:38:LYS:HD3	1:A:122:ASN:OD1	2.14	0.47
1:B:1093:VAL:CG2	1:B:1188:GLU:OE2	2.62	0.47
1:C:2090:PHE:O	1:C:2093:VAL:N	2.48	0.47
1:D:3027:PHE:CD1	1:D:3027:PHE:C	2.87	0.47
1:A:121:PHE:HB2	1:A:132:TRP:CH2	2.50	0.47
1:A:133:GLU:CA	1:A:133:GLU:OE2	2.62	0.47
1:A:43:TRP:HZ3	1:A:187:LEU:HB2	1.77	0.47
1:E:4130:SER:OG	1:E:4169:TRP:NE1	2.47	0.47
1:E:4161:ALA:HA	1:E:4179:ASN:O	2.15	0.47
1:C:2070:GLN:NE2	1:C:2179:ASN:OD1	2.48	0.46
1:D:3055:GLY:C	1:D:3057:ASP:H	2.17	0.46
1:D:3134:TYR:C	1:D:3135:ARG:HD2	2.36	0.46
1:C:2058:LEU:O	1:C:2059:SER:HB2	2.15	0.46
1:D:3104:LEU:C	1:D:3106:THR:H	2.18	0.46
1:E:4087:HIS:CD2	1:E:4096:LEU:H	2.25	0.46
1:A:7:PHE:CE1	1:A:154:VAL:HG12	2.49	0.46
1:A:74:GLU:O	1:A:75:VAL:C	2.53	0.46
1:B:1068:ILE:HD12	1:B:1182:VAL:HB	1.97	0.46
1:A:34:LEU:O	1:A:35:GLU:HB2	2.15	0.46
1:A:78:MET:HE1	1:A:159:ILE:CG2	2.46	0.46
1:D:3067:THR:HG22	1:D:3068:ILE:N	2.29	0.46
1:D:3107:PHE:C	1:D:3110:LEU:HG	2.36	0.46
1:D:3111:GLU:O	1:D:3113:GLU:N	2.48	0.46
1:A:194:GLY:O	1:A:195:PHE:C	2.53	0.46
1:B:1163:ILE:HD11	1:B:1178:LYS:CE	2.46	0.46
1:C:2087:HIS:CE1	1:C:2095:ASP:HA	2.50	0.46
1:D:3056:GLU:O	1:D:3056:GLU:HG3	2.16	0.46
1:C:2098:LYS:HE2	1:C:2102:ILE:HD11	1.97	0.46
1:D:3121:PHE:HE1	1:D:3130:SER:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3119:LEU:O	1:D:3132:TRP:HZ3	1.99	0.46
1:E:4058:LEU:HB2	1:E:4195:PHE:CD1	2.50	0.46
1:E:4094:VAL:HG13	1:E:4099:LEU:CD2	2.46	0.46
1:A:99:LEU:HD23	1:A:99:LEU:H	1.81	0.46
1:C:2076:GLY:N	1:C:2174:SER:O	2.45	0.46
1:A:130:SER:HG	1:A:169:TRP:HE1	1.64	0.46
1:A:41:PHE:HE1	1:A:43:TRP:CD2	2.33	0.46
1:C:2086:LEU:O	1:C:2090:PHE:N	2.48	0.46
1:C:2090:PHE:O	1:C:2093:VAL:HG12	2.16	0.46
1:C:2103:ILE:O	1:C:2103:ILE:CG2	2.63	0.46
1:C:2120:GLN:NE2	1:C:2121:PHE:O	2.44	0.46
1:C:2127:LYS:HB2	1:C:2129:ASN:OD1	2.15	0.46
1:D:3118:PHE:O	1:D:3135:ARG:HD3	2.16	0.46
1:E:4128:LYS:HG3	1:E:4164:GLU:OE1	2.15	0.46
1:E:4043:TRP:CZ3	1:E:4187:LEU:HB2	2.51	0.46
1:B:1050:ILE:CG2	1:B:1060:PHE:HB2	2.46	0.46
1:B:1161:ALA:HB3	1:B:1169:TRP:CH2	2.51	0.46
1:C:2036:GLN:C	1:C:2038:LYS:H	2.19	0.46
1:C:2058:LEU:HD12	1:C:2195:PHE:CZ	2.51	0.46
1:D:3036:GLN:O	1:D:3037:ASP:HB3	2.16	0.46
1:B:1008:GLN:NE2	1:B:1134:TYR:OH	2.49	0.46
1:C:2022:ILE:O	1:C:2025:LEU:HB3	2.15	0.46
1:D:3111:GLU:C	1:D:3113:GLU:N	2.68	0.46
1:A:82:ILE:HG21	1:A:157:ILE:CD1	2.46	0.45
1:A:18:ILE:HD12	1:D:3146:ALA:HB2	1.97	0.45
1:A:15:GLU:HA	1:A:18:ILE:HD12	1.97	0.45
1:C:2036:GLN:HG3	1:C:2036:GLN:O	2.16	0.45
1:A:93:VAL:HG23	1:A:188:GLU:OE1	2.16	0.45
1:A:36:GLN:NE2	1:A:36:GLN:HA	2.32	0.45
1:A:62:LYS:HG2	1:A:63:TYR:N	2.31	0.45
1:C:2043:TRP:CB	1:C:2044:PRO:HD3	2.46	0.45
1:C:2146:ALA:HA	1:E:4015:GLU:HB3	1.99	0.45
1:D:3132:TRP:HD1	1:D:3169:TRP:CD2	2.33	0.45
1:E:4178:LYS:HB3	1:E:4180:PHE:CZ	2.52	0.45
1:A:82:ILE:HD13	1:A:157:ILE:HD13	1.99	0.45
1:A:74:GLU:O	1:A:77:ALA:N	2.39	0.45
1:C:2099:LEU:CD1	1:C:2138:PHE:CZ	2.99	0.45
1:D:3053:TYR:CE2	1:D:3058:LEU:HB3	2.51	0.45
1:E:4034:LEU:HG	1:E:4035:GLU:N	2.31	0.45
1:A:132:TRP:O	1:A:158:LEU:HA	2.16	0.45
1:A:63:TYR:O	1:A:64:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:C	1:A:128:LYS:H	2.20	0.45
1:D:3015:GLU:O	1:D:3018:ILE:HG12	2.17	0.45
1:E:4013:LEU:HD12	1:E:4013:LEU:O	2.16	0.45
1:C:2031:TYR:O	1:C:2042:ASP:HB3	2.17	0.45
1:D:3066:SER:HB3	1:D:3085:PHE:CE2	2.51	0.45
1:D:3068:ILE:O	1:D:3181:ALA:HA	2.16	0.45
1:D:3107:PHE:HA	1:D:3110:LEU:CD2	2.47	0.45
1:E:4034:LEU:HD12	1:E:4038:LYS:O	2.17	0.45
1:A:68:ILE:HD13	1:A:81:LYS:HD2	1.98	0.45
1:C:2030:LYS:HG3	1:C:2030:LYS:O	2.17	0.45
1:E:4015:GLU:O	1:E:4019:PRO:HD3	2.17	0.45
1:B:1126:VAL:C	1:B:1128:LYS:N	2.70	0.45
1:C:2165:GLU:O	1:C:2167:THR:N	2.49	0.45
1:C:2179:ASN:H	1:C:2179:ASN:HD22	1.62	0.45
1:D:3090:PHE:C	1:D:3092:ALA:H	2.20	0.45
1:A:155:THR:HG22	1:A:156:THR:N	2.31	0.45
1:A:161:ALA:HB2	1:A:180:PHE:HD1	1.81	0.45
1:A:90:PHE:CE2	1:A:186:ALA:HB3	2.52	0.45
1:A:8:GLN:HE21	1:A:118:PHE:HZ	1.65	0.45
1:A:86:LEU:HB3	1:A:94:VAL:HG21	1.98	0.45
1:B:1087:HIS:HA	1:B:1094:VAL:HG23	1.98	0.45
1:B:1144:ASP:O	1:B:1147:PRO:HD3	2.17	0.45
1:C:2161:ALA:HB3	1:C:2163:ILE:HG12	1.98	0.45
1:D:3129:ASN:HA	1:D:3161:ALA:O	2.17	0.45
1:E:4015:GLU:O	1:E:4017:LEU:N	2.50	0.45
1:E:4036:GLN:O	1:E:4038:LYS:HG3	2.16	0.45
1:E:4113:GLU:O	1:E:4114:SER:C	2.55	0.45
1:E:4060:PHE:HA	1:E:4189:LEU:HD23	1.98	0.45
1:C:2096:LEU:HD22	1:C:2097:SER:H	1.76	0.44
1:A:36:GLN:HB2	1:A:38:LYS:HE2	1.99	0.44
1:C:2074:GLU:CD	1:C:2074:GLU:H	2.21	0.44
1:C:2142:PHE:HZ	1:E:4022:ILE:CD1	2.27	0.44
1:D:3069:ASN:O	1:D:3071:GLN:HG2	2.18	0.44
1:D:3013:LEU:HG	1:D:3139:SER:O	2.17	0.44
1:A:74:GLU:O	1:A:77:ALA:CB	2.65	0.44
1:B:1107:PHE:C	1:B:1109:ASN:H	2.20	0.44
1:B:1155:THR:HB	1:B:1186:ALA:HB2	1.99	0.44
1:A:126:VAL:C	1:A:128:LYS:N	2.71	0.44
1:A:46:PHE:CG	1:A:46:PHE:O	2.70	0.44
1:A:75:VAL:C	1:A:77:ALA:N	2.71	0.44
1:B:1086:LEU:C	1:B:1088:ASP:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1093:VAL:HG21	1:B:1188:GLU:CD	2.38	0.44
1:B:1136:VAL:HG13	1:B:1155:THR:HG23	1.99	0.44
1:C:2178:LYS:O	1:C:2180:PHE:CD2	2.69	0.44
1:D:3062:LYS:HE3	1:D:3064:ASP:HB2	1.98	0.44
1:C:2128:LYS:O	1:C:2164:GLU:OE1	2.36	0.44
1:B:1111:GLU:HB3	1:D:3069:ASN:OD1	2.17	0.44
1:D:3084:LYS:O	1:D:3088:ASP:N	2.46	0.44
1:D:3150:PHE:CZ	1:D:3191:VAL:HG11	2.52	0.44
1:A:13:LEU:HD12	1:A:13:LEU:C	2.37	0.44
1:B:1020:SER:OG	1:B:1194:GLY:N	2.48	0.44
1:C:2109:ASN:HD22	1:C:2109:ASN:HA	1.49	0.44
1:D:3084:LYS:O	1:D:3087:HIS:HB3	2.18	0.44
1:E:4012:GLN:NE2	1:E:4141:PRO:CD	2.81	0.44
1:B:1043:TRP:HZ3	1:B:1187:LEU:HB2	1.83	0.44
1:B:1111:GLU:HB3	1:D:3069:ASN:ND2	2.32	0.44
1:C:2046:PHE:O	1:C:2049:ALA:HB3	2.18	0.44
1:D:3015:GLU:C	1:D:3017:LEU:N	2.68	0.44
1:B:1044:PRO:O	1:B:1047:LYS:HB2	2.17	0.44
1:D:3015:GLU:HA	1:D:3018:ILE:CG1	2.47	0.43
1:E:4060:PHE:C	1:E:4060:PHE:CD2	2.91	0.43
1:C:2057:ASP:O	1:C:2191:VAL:HA	2.19	0.43
1:D:3171:GLY:C	1:D:3172:LEU:HD12	2.38	0.43
1:A:73:GLN:HE21	1:A:180:PHE:HB2	1.82	0.43
1:C:2057:ASP:N	1:C:2057:ASP:OD2	2.51	0.43
1:D:3107:PHE:CA	1:D:3110:LEU:HG	2.48	0.43
1:D:3174:SER:O	1:D:3175:SER:HB2	2.18	0.43
1:E:4053:TYR:CE2	1:E:4058:LEU:HB3	2.53	0.43
1:A:43:TRP:CH2	1:A:187:LEU:HB2	2.53	0.43
1:A:36:GLN:HE21	1:A:36:GLN:HA	1.84	0.43
1:D:3082:ILE:HD11	1:D:3157:ILE:HD13	2.00	0.43
1:D:3093:VAL:HG13	1:D:3140:VAL:HG13	1.99	0.43
1:D:3135:ARG:O	1:D:3136:VAL:HG13	2.18	0.43
1:E:4126:VAL:HG23	1:E:4127:LYS:H	1.83	0.43
1:B:1021:SER:O	1:B:1024:VAL:HB	2.17	0.43
1:E:4024:VAL:HG21	1:E:4191:VAL:HG21	1.99	0.43
1:C:2029:GLY:C	1:C:2031:TYR:H	2.22	0.43
1:C:2128:LYS:HZ3	1:D:3098:LYS:NZ	2.10	0.43
1:A:40:TYR:HD1	1:A:133:GLU:HG2	1.83	0.43
1:A:67:THR:OG1	1:A:183:GLN:NE2	2.52	0.43
1:C:2146:ALA:HA	1:E:4015:GLU:OE2	2.17	0.43
1:E:4126:VAL:C	1:E:4128:LYS:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLY:C	1:A:145:ASN:H	2.22	0.43
1:A:53:TYR:CE2	1:A:58:LEU:HB3	2.53	0.43
1:A:60:PHE:C	1:A:60:PHE:CD2	2.92	0.43
1:A:78:MET:HA	1:A:81:LYS:NZ	2.33	0.43
1:A:87:HIS:HA	1:A:94:VAL:HB	2.00	0.43
1:B:1133:GLU:HG2	1:B:1135:ARG:HH12	1.84	0.43
1:D:3138:PHE:HB2	1:D:3153:LEU:HB2	2.00	0.43
1:E:4110:LEU:O	1:E:4111:GLU:C	2.57	0.43
1:B:1073:GLN:NE2	1:B:1081:LYS:HE2	2.34	0.43
1:C:2023:GLN:HA	1:C:2026:LYS:HG3	2.00	0.43
1:C:2144:ASP:O	1:C:2147:PRO:HD3	2.18	0.43
1:D:3007:PHE:O	1:D:3009:PRO:CD	2.67	0.43
1:D:3100:ALA:O	1:D:3104:LEU:HB2	2.18	0.43
1:E:4008:GLN:NE2	2:E:5012:HOH:O	2.51	0.43
1:B:1086:LEU:HB3	1:B:1094:VAL:HG21	2.01	0.43
1:C:2061:ASP:O	1:C:2062:LYS:HB2	2.19	0.43
1:E:4129:ASN:OD1	1:E:4130:SER:N	2.52	0.43
1:A:107:PHE:CZ	1:A:159:ILE:HD13	2.54	0.42
1:A:110:LEU:O	1:A:111:GLU:C	2.57	0.42
1:A:40:TYR:CD1	1:A:133:GLU:HG2	2.54	0.42
1:A:161:ALA:O	1:A:163:ILE:N	2.52	0.42
1:B:1026:LYS:O	1:B:1026:LYS:HG2	2.18	0.42
1:D:3006:VAL:O	1:D:3118:PHE:HB3	2.19	0.42
1:E:4025:LEU:CD1	1:E:4137:LEU:HD23	2.48	0.42
1:B:1134:TYR:HB3	1:B:1157:ILE:HB	2.01	0.42
1:B:1010:VAL:HG11	1:B:1138:PHE:HE1	1.83	0.42
1:C:2071:GLN:HE22	1:C:2073:GLN:CD	2.23	0.42
1:C:2119:LEU:HA	1:C:2119:LEU:HD23	1.80	0.42
1:D:3106:THR:O	1:D:3110:LEU:HD23	2.19	0.42
1:A:107:PHE:CE1	1:A:159:ILE:CD1	3.02	0.42
1:A:126:VAL:HG23	1:A:127:LYS:N	2.34	0.42
1:A:130:SER:HG	1:A:169:TRP:HZ2	1.64	0.42
1:A:163:ILE:CG2	1:A:168:GLY:HA3	2.49	0.42
1:A:33:LYS:HG2	1:A:40:TYR:O	2.19	0.42
1:A:41:PHE:HZ	1:A:46:PHE:CD2	2.36	0.42
1:D:3110:LEU:O	1:D:3114:SER:N	2.52	0.42
1:D:3124:ASN:C	1:D:3126:VAL:H	2.23	0.42
1:E:4053:TYR:CE2	1:E:4055:GLY:HA3	2.54	0.42
1:B:1034:LEU:HD23	1:B:1039:ALA:HB2	2.01	0.42
1:B:1159:ILE:CD1	1:B:1159:ILE:N	2.80	0.42
1:C:2071:GLN:HE21	1:C:2071:GLN:CA	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2136:VAL:HG12	1:C:2137:LEU:H	1.83	0.42
1:D:3061:ASP:HB3	1:D:3188:GLU:HG2	2.01	0.42
1:D:3140:VAL:HG23	1:D:3141:PRO:O	2.18	0.42
1:D:3050:ILE:HD11	1:D:3187:LEU:HD11	2.00	0.42
1:E:4015:GLU:C	1:E:4017:LEU:N	2.72	0.42
1:E:4096:LEU:HB3	1:E:4097:SER:H	1.49	0.42
1:E:4090:PHE:CE2	1:E:4186:ALA:HB3	2.55	0.42
1:E:4058:LEU:CD2	1:E:4191:VAL:HG22	2.49	0.42
1:A:158:LEU:O	1:A:182:VAL:HA	2.19	0.42
1:C:2027:PHE:HB2	1:C:2198:PRO:HD2	2.02	0.42
1:C:2112:GLU:CD	1:C:2112:GLU:H	2.22	0.42
1:D:3150:PHE:CZ	1:D:3191:VAL:HG13	2.55	0.42
1:E:4062:LYS:HZ1	1:E:4064:ASP:HB2	1.82	0.42
1:E:4066:SER:HB2	1:E:4085:PHE:CD1	2.54	0.42
1:E:4079:VAL:HG13	1:E:4103:ILE:CG2	2.50	0.42
1:C:2171:GLY:O	1:C:2172:LEU:C	2.58	0.42
1:D:3046:PHE:O	1:D:3049:ALA:HB3	2.20	0.42
1:D:3093:VAL:HG21	1:D:3153:LEU:HD21	2.02	0.42
1:B:1018:ILE:O	1:B:1019:PRO:C	2.57	0.42
1:B:1161:ALA:HA	1:B:1179:ASN:O	2.20	0.42
1:B:1188:GLU:O	1:B:1189:LEU:HD12	2.19	0.42
1:C:2114:SER:C	1:C:2116:SER:H	2.23	0.42
1:A:24:VAL:CG2	1:A:191:VAL:HG21	2.49	0.42
1:D:3023:GLN:HB3	1:D:3195:PHE:CD2	2.54	0.42
1:E:4107:PHE:CZ	1:E:4159:ILE:HD13	2.54	0.42
1:A:142:PHE:HB2	1:A:149:TYR:O	2.20	0.42
1:E:4006:VAL:O	1:E:4135:ARG:NE	2.48	0.42
1:A:106:THR:HG23	1:A:113:GLU:HG2	2.02	0.42
1:A:87:HIS:ND1	1:A:87:HIS:C	2.74	0.42
1:C:2007:PHE:CE2	1:C:2028:SER:HB3	2.55	0.42
1:C:2046:PHE:CZ	1:C:2050:ILE:HD11	2.54	0.42
1:C:2121:PHE:CZ	1:C:2130:SER:HB2	2.55	0.42
1:B:1058:LEU:C	1:B:1058:LEU:HD23	2.41	0.41
1:C:2047:LYS:C	1:C:2049:ALA:H	2.23	0.41
1:C:2140:VAL:HG23	1:C:2141:PRO:O	2.20	0.41
1:E:4058:LEU:HD21	1:E:4189:LEU:HD13	2.01	0.41
1:A:107:PHE:HA	1:A:110:LEU:HD23	2.00	0.41
1:A:126:VAL:O	1:A:128:LYS:N	2.53	0.41
1:A:129:ASN:OD1	1:A:129:ASN:C	2.58	0.41
1:A:136:VAL:HG13	1:A:155:THR:HB	2.02	0.41
1:B:1031:TYR:O	1:B:1042:ASP:N	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2091:ALA:C	1:C:2093:VAL:N	2.71	0.41
1:C:2187:LEU:O	1:C:2187:LEU:HD23	2.20	0.41
1:D:3121:PHE:CG	1:D:3122:ASN:N	2.88	0.41
1:E:4015:GLU:C	1:E:4017:LEU:H	2.23	0.41
1:B:1082:ILE:HG21	1:B:1157:ILE:HD13	2.03	0.41
1:C:2121:PHE:CG	1:C:2122:ASN:N	2.88	0.41
1:C:2107:PHE:CE1	1:C:2159:ILE:HD13	2.56	0.41
1:D:3129:ASN:ND2	1:D:3162:ASP:HA	2.36	0.41
1:A:85:PHE:O	1:A:89:ALA:N	2.49	0.41
1:C:2079:VAL:HG11	1:C:2104:LEU:HB2	2.02	0.41
1:C:2102:ILE:N	1:C:2102:ILE:CD1	2.82	0.41
1:D:3073:GLN:HE21	1:D:3078:MET:HA	1.84	0.41
1:E:4068:ILE:HG22	1:E:4068:ILE:O	2.20	0.41
1:B:1121:PHE:CE1	1:B:1130:SER:HB2	2.55	0.41
1:C:2128:LYS:HZ2	1:D:3098:LYS:NZ	2.17	0.41
1:E:4093:VAL:HG13	1:E:4140:VAL:CG2	2.49	0.41
1:A:13:LEU:HD13	1:A:17:LEU:HB2	2.03	0.41
1:B:1061:ASP:OD1	1:B:1062:LYS:HE2	2.21	0.41
1:B:1090:PHE:HD1	1:B:1188:GLU:HG3	1.85	0.41
1:C:2047:LYS:O	1:C:2050:ILE:N	2.53	0.41
1:C:2133:GLU:OE2	1:C:2135:ARG:CG	2.68	0.41
1:D:3130:SER:CB	1:D:3169:TRP:HE1	2.32	0.41
1:D:3153:LEU:HD21	1:D:3188:GLU:HB2	1.98	0.41
1:D:3007:PHE:HD1	1:D:3136:VAL:H	1.69	0.41
1:D:3008:GLN:HE21	1:D:3008:GLN:HB3	1.71	0.41
1:D:3110:LEU:HD22	1:D:3119:LEU:HD13	2.03	0.41
1:D:3025:LEU:HD13	1:D:3137:LEU:HD12	2.02	0.41
1:E:4086:LEU:O	1:E:4087:HIS:C	2.57	0.41
1:E:4127:LYS:O	1:E:4128:LYS:C	2.58	0.41
1:B:1020:SER:O	1:B:1023:GLN:HB2	2.21	0.41
1:D:3022:ILE:HG22	1:D:3022:ILE:O	2.20	0.41
1:D:3058:LEU:HD23	1:D:3058:LEU:C	2.41	0.41
1:D:3110:LEU:O	1:D:3113:GLU:C	2.58	0.41
1:D:3135:ARG:CD	1:D:3135:ARG:N	2.82	0.41
1:E:4120:GLN:HB3	1:E:4133:GLU:CB	2.46	0.41
1:D:3107:PHE:HA	1:D:3110:LEU:HD21	2.03	0.41
1:D:3132:TRP:HD1	1:D:3169:TRP:CE3	2.39	0.41
1:D:3032:LEU:HD11	1:D:3135:ARG:HH12	1.85	0.41
1:A:178:LYS:HB2	1:A:180:PHE:CE2	2.56	0.41
1:D:3030:LYS:O	1:D:3031:TYR:CD2	2.74	0.41
1:E:4033:LYS:O	1:E:4033:LYS:CG	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4064:ASP:OD1	1:E:4065:GLN:N	2.54	0.41
1:A:110:LEU:HD11	1:A:132:TRP:CE2	2.56	0.41
1:A:169:TRP:O	1:A:172:LEU:HD12	2.21	0.41
1:A:98:LYS:HE2	1:C:2044:PRO:HG2	2.02	0.41
1:C:2138:PHE:O	1:C:2152:SER:HA	2.21	0.41
1:E:4096:LEU:O	1:E:4099:LEU:CD2	2.69	0.41
1:E:4114:SER:C	1:E:4116:SER:N	2.74	0.41
1:A:78:MET:HG3	1:A:79:VAL:N	2.36	0.40
1:D:3006:VAL:HG21	1:D:3029:GLY:HA3	2.03	0.40
1:D:3128:LYS:C	1:D:3129:ASN:HD22	2.24	0.40
1:E:4043:TRP:HZ3	1:E:4187:LEU:CB	2.34	0.40
1:A:175:SER:O	1:A:176:THR:C	2.60	0.40
1:B:1165:GLU:C	1:B:1167:THR:N	2.74	0.40
1:C:2041:PHE:HZ	1:C:2046:PHE:CG	2.39	0.40
1:C:2043:TRP:O	1:C:2044:PRO:C	2.59	0.40
1:C:2062:LYS:CG	1:C:2063:TYR:N	2.84	0.40
1:C:2158:LEU:O	1:C:2182:VAL:HA	2.20	0.40
1:D:3065:GLN:HG3	1:D:3185:ASP:OD2	2.21	0.40
1:E:4032:LEU:HD22	1:E:4039:ALA:HB1	2.03	0.40
1:B:1136:VAL:HG21	1:B:1138:PHE:CZ	2.56	0.40
1:C:2031:TYR:CE1	1:C:2049:ALA:HB2	2.56	0.40
1:D:3111:GLU:HG3	1:D:3170:TRP:HE1	1.85	0.40
1:E:4133:GLU:CA	1:E:4133:GLU:OE2	2.69	0.40
1:E:4166:LYS:O	1:E:4168:GLY:N	2.54	0.40
1:A:60:PHE:CD1	1:A:187:LEU:HD21	2.56	0.40
1:A:5:ASN:HA	1:A:5:ASN:HD22	1.56	0.40
1:A:94:VAL:HG13	1:A:99:LEU:HD13	2.02	0.40
1:B:1050:ILE:HD12	1:B:1189:LEU:HD11	2.03	0.40
1:B:1125:ASN:N	1:B:1125:ASN:HD22	2.18	0.40
1:B:1148:SER:O	1:B:1192:LYS:HA	2.22	0.40
1:D:3078:MET:O	1:D:3080:ASP:N	2.54	0.40
1:D:3152:SER:HB2	1:D:3189:LEU:CD1	2.51	0.40
1:B:1146:ALA:O	1:B:1149:TYR:N	2.43	0.40
1:B:1070:GLN:HA	1:B:1180:PHE:O	2.22	0.40
1:B:1184:ILE:O	1:B:1184:ILE:HG12	2.20	0.40
1:B:1150:PHE:CZ	1:B:1191:VAL:HB	2.56	0.40
1:C:2072:SER:O	1:C:2177:LYS:HD3	2.21	0.40
1:D:3087:HIS:HD2	1:D:3096:LEU:CB	2.34	0.40
1:E:4078:MET:HG3	1:E:4079:VAL:N	2.37	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	192/199 (96%)	153 (80%)	29 (15%)	10 (5%)	2	17
1	B	192/199 (96%)	153 (80%)	26 (14%)	13 (7%)	1	10
1	C	192/199 (96%)	139 (72%)	29 (15%)	24 (12%)	0	2
1	D	192/199 (96%)	138 (72%)	35 (18%)	19 (10%)	1	3
1	E	182/199 (92%)	148 (81%)	30 (16%)	4 (2%)	7	39
All	All	950/995 (96%)	731 (77%)	149 (16%)	70 (7%)	1	8

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	B	1116	SER
1	C	2027	PHE
1	C	2036	GLN
1	C	2093	VAL
1	C	2096	LEU
1	C	2146	ALA
1	C	2174	SER
1	C	2175	SER
1	D	3069	ASN
1	D	3091	ALA
1	D	3096	LEU
1	D	3175	SER
1	E	4035	GLU
1	A	52	ASN
1	A	76	GLY
1	A	162	ASP
1	B	1052	ASN
1	B	1108	THR
1	B	1126	VAL
1	C	2015	GLU

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Mol	Chain	Res	Type
1	C	2028	SER
1	C	2092	ALA
1	C	2111	GLU
1	C	2166	LYS
1	D	3016	ASP
1	D	3035	GLU
1	D	3075	VAL
1	D	3079	VAL
1	D	3093	VAL
1	D	3111	GLU
1	E	4115	SER
1	A	35	GLU
1	A	70	GLN
1	B	1087	HIS
1	B	1091	ALA
1	B	1125	ASN
1	B	1127	LYS
1	C	2016	ASP
1	C	2059	SER
1	C	2084	LYS
1	C	2097	SER
1	C	2100	ALA
1	C	2172	LEU
1	C	2176	THR
1	D	3008	GLN
1	D	3056	GLU
1	D	3070	GLN
1	D	3164	GLU
1	A	93	VAL
1	B	1034	LEU
1	B	1058	LEU
1	B	1164	GLU
1	B	1166	LYS
1	C	2048	THR
1	C	2145	ASN
1	D	3015	GLU
1	D	3097	SER
1	D	3144	ASP
1	A	34	LEU
1	A	53	TYR
1	A	113	GLU
1	C	2091	ALA

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Mol	Chain	Res	Type
1	D	3112	GLU
1	C	2026	LYS
1	E	4016	ASP
1	E	4052	ASN
1	C	2117	GLY
1	D	3019	PRO
1	B	1093	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/175 (98%)	153 (90%)	18 (10%)	7	31
1	B	171/175 (98%)	160 (94%)	11 (6%)	19	56
1	C	171/175 (98%)	155 (91%)	16 (9%)	9	36
1	D	171/175 (98%)	155 (91%)	16 (9%)	9	36
1	E	164/175 (94%)	148 (90%)	16 (10%)	9	34
All	All	848/875 (97%)	771 (91%)	77 (9%)	10	37

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	12	GLN
1	A	16	ASP
1	A	51	ASP
1	A	52	ASN
1	A	61	ASP
1	A	80	ASP
1	A	95	ASP
1	A	99	LEU
1	A	110	LEU
1	A	113	GLU
1	A	125	ASN

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Mol	Chain	Res	Type
1	A	154	VAL
1	A	159	ILE
1	A	160	THR
1	A	170	TRP
1	A	172	LEU
1	A	183	GLN
1	B	1005	ASN
1	B	1009	PRO
1	B	1030	LYS
1	B	1062	LYS
1	B	1133	GLU
1	B	1155	THR
1	B	1170	TRP
1	B	1173	THR
1	B	1184	ILE
1	B	1185	ASP
1	B	1188	GLU
1	C	2019	PRO
1	C	2048	THR
1	C	2057	ASP
1	C	2071	GLN
1	C	2074	GLU
1	C	2085	PHE
1	C	2096	LEU
1	C	2105	ASN
1	C	2109	ASN
1	C	2112	GLU
1	C	2136	VAL
1	C	2140	VAL
1	C	2152	SER
1	C	2167	THR
1	C	2170	TRP
1	C	2185	ASP
1	D	3011	ASP
1	D	3027	PHE
1	D	3030	LYS
1	D	3051	ASP
1	D	3086	LEU
1	D	3096	LEU
1	D	3107	PHE
1	D	3123	THR
1	D	3132	TRP

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Mol	Chain	Res	Type
1	D	3136	VAL
1	D	3140	VAL
1	D	3155	THR
1	D	3177	LYS
1	D	3188	GLU
1	D	3189	LEU
1	D	3192	LYS
1	E	4005	ASN
1	E	4012	GLN
1	E	4016	ASP
1	E	4051	ASP
1	E	4052	ASN
1	E	4096	LEU
1	E	4099	LEU
1	E	4105	ASN
1	E	4110	LEU
1	E	4112	GLU
1	E	4113	GLU
1	E	4118	PHE
1	E	4159	ILE
1	E	4170	TRP
1	E	4182	VAL
1	E	4183	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	12	GLN
1	A	36	GLN
1	A	52	ASN
1	A	65	GLN
1	A	105	ASN
1	A	124	ASN
1	A	183	GLN
1	B	1008	GLN
1	B	1036	GLN
1	B	1052	ASN
1	B	1073	GLN
1	B	1087	HIS
1	B	1125	ASN
1	B	1145	ASN

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Mol	Chain	Res	Type
1	C	2008	GLN
1	C	2036	GLN
1	C	2052	ASN
1	C	2065	GLN
1	C	2070	GLN
1	C	2071	GLN
1	C	2073	GLN
1	C	2109	ASN
1	C	2122	ASN
1	C	2179	ASN
1	D	3008	GLN
1	D	3052	ASN
1	D	3065	GLN
1	D	3073	GLN
1	D	3087	HIS
1	D	3120	GLN
1	D	3122	ASN
1	D	3124	ASN
1	D	3129	ASN
1	D	3183	GLN
1	E	4005	ASN
1	E	4012	GLN
1	E	4036	GLN
1	E	4052	ASN
1	E	4065	GLN
1	E	4105	ASN
1	E	4124	ASN
1	E	4183	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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	194/199 (97%)	-0.22	1 (0%) 90 86	22, 56, 89, 108	0
1	B	194/199 (97%)	-0.11	4 (2%) 63 49	29, 59, 96, 126	0
1	C	194/199 (97%)	0.05	6 (3%) 49 33	22, 66, 103, 116	0
1	D	194/199 (97%)	0.38	20 (10%) 6 4	23, 84, 134, 155	0
1	E	186/199 (93%)	1.94	69 (37%) 0 0	70, 149, 185, 191	0
All	All	962/995 (96%)	0.39	100 (10%) 6 4	22, 71, 173, 191	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4177	LYS	7.8
1	E	4176	THR	7.8
1	E	4094	VAL	7.7
1	E	4096	LEU	7.5
1	E	4083	ALA	6.1
1	E	4039	ALA	6.1
1	E	4163	ILE	5.6
1	E	4027	PHE	5.5
1	E	4037	ASP	5.5
1	E	4095	ASP	5.4
1	E	4130	SER	5.4
1	E	4099	LEU	5.4
1	D	3166	LYS	5.2
1	E	4129	ASN	5.2
1	D	3165	GLU	5.0
1	D	3170	TRP	4.9
1	E	4115	SER	4.7
1	E	4165	GLU	4.5
1	E	4081	LYS	4.5
1	E	4174	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	4175	SER	4.4
1	E	4079	VAL	4.4
1	E	4031	TYR	4.4
1	E	4164	GLU	4.2
1	D	3164	GLU	4.2
1	E	4098	LYS	4.0
1	E	4038	LYS	4.0
1	D	3171	GLY	3.9
1	D	3125	ASN	3.7
1	E	4128	LYS	3.7
1	E	4107	PHE	3.6
1	E	4084	LYS	3.6
1	D	3126	VAL	3.6
1	E	4049	ALA	3.5
1	E	4126	VAL	3.4
1	E	4167	THR	3.4
1	E	4111	GLU	3.4
1	E	4040	TYR	3.4
1	E	4125	ASN	3.4
1	E	4097	SER	3.3
1	E	4108	THR	3.3
1	D	3128	LYS	3.2
1	E	4077	ALA	3.2
1	D	3179	ASN	3.2
1	E	4170	TRP	3.1
1	E	4089	ALA	3.1
1	E	4105	ASN	3.0
1	E	4100	ALA	3.0
1	E	4087	HIS	3.0
1	E	4198	PRO	3.0
1	E	4116	SER	2.9
1	E	4127	LYS	2.9
1	E	4181	ALA	2.9
1	B	1045	GLY	2.8
1	D	3169	TRP	2.8
1	E	4120	GLN	2.8
1	E	4067	THR	2.8
1	E	4135	ARG	2.8
1	D	3167	THR	2.8
1	C	2036	GLN	2.8
1	E	4033	LYS	2.8
1	E	4085	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	4078	MET	2.7
1	C	2034	LEU	2.7
1	E	4121	PHE	2.7
1	E	4052	ASN	2.7
1	E	4035	GLU	2.6
1	E	4086	LEU	2.6
1	E	4187	LEU	2.6
1	B	1054	THR	2.6
1	E	4044	PRO	2.5
1	E	4180	PHE	2.5
1	E	4133	GLU	2.5
1	E	4093	VAL	2.5
1	D	3097	SER	2.5
1	D	3111	GLU	2.5
1	E	4162	ASP	2.5
1	C	2037	ASP	2.4
1	B	1128	LYS	2.4
1	E	4104	LEU	2.4
1	C	2048	THR	2.4
1	D	3096	LEU	2.4
1	D	3070	GLN	2.4
1	E	4048	THR	2.4
1	A	54	THR	2.3
1	E	4156	THR	2.3
1	B	1164	GLU	2.3
1	D	3036	GLN	2.3
1	E	4080	ASP	2.2
1	C	2052	ASN	2.2
1	E	4008	GLN	2.2
1	E	4054	THR	2.2
1	D	3037	ASP	2.2
1	E	4056	GLU	2.2
1	E	4068	ILE	2.2
1	E	4007	PHE	2.1
1	D	3072	SER	2.1
1	D	3035	GLU	2.1
1	D	3080	ASP	2.0
1	C	2112	GLU	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.