



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:12 AM UTC

PDB ID : 1PP6 / pdb\_00001pp6  
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.

The types of validation reports are described at

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

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

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

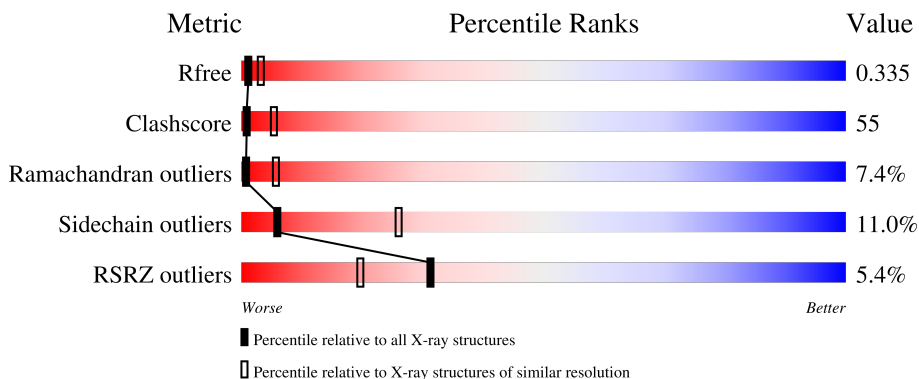
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	199	 28% 54% 15% . .
1	B	199	 28% 57% 13% .
1	C	199	 25% 53% 19% . .
1	D	199	 2% 24% 56% 15% . .
1	E	199	 23% 30% 53% 10% . 7%

## 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
			Total	C	N	O	S			
1	A	194	1547	1004	241	301	1	0	0	0
1	B	194	1547	1004	241	301	1	0	0	0
1	C	194	1547	1004	241	301	1	0	0	0
1	D	194	1547	1004	241	301	1	0	0	0
1	E	186	1486	970	229	286	1	0	0	0

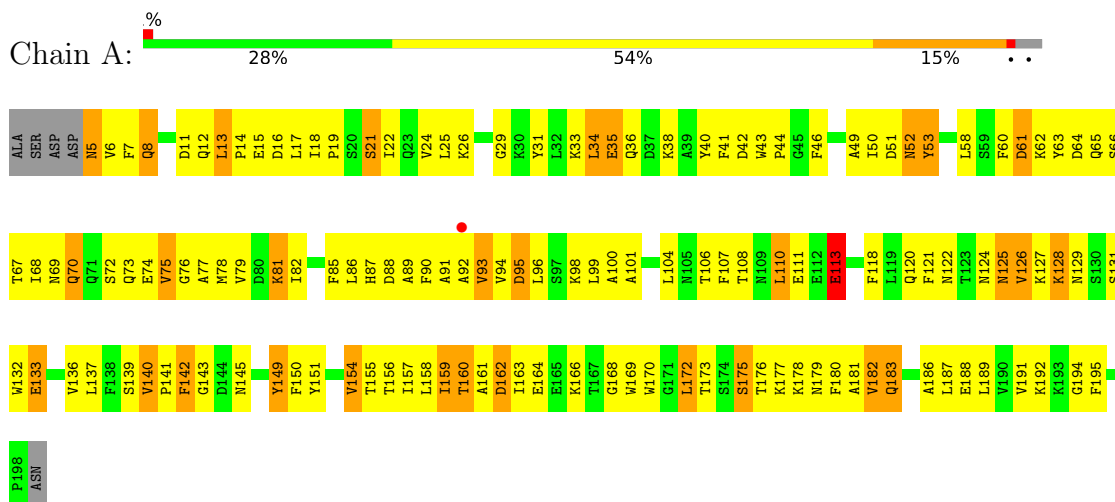
- Molecule 2 is water.

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

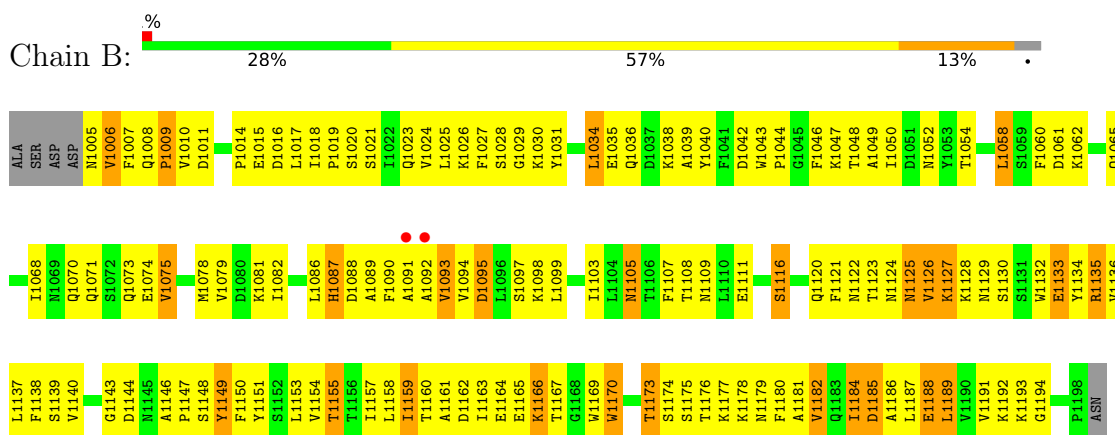
### 3 Residue-property plots

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

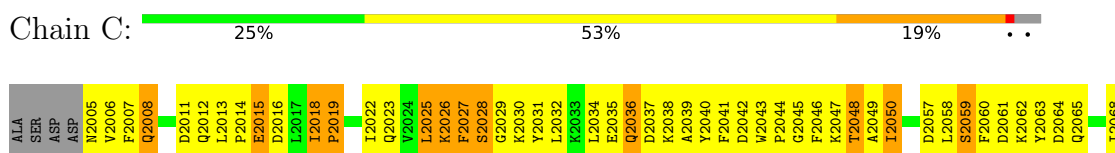
- Molecule 1: Volvatoxin A2



- Molecule 1: Volvatoxin A2



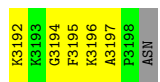
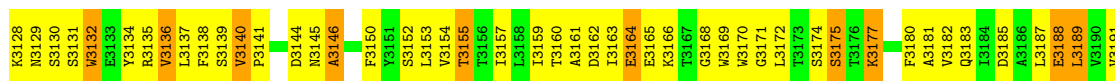
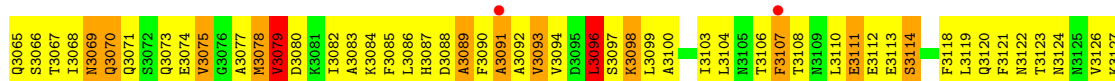
- Molecule 1: Volvatoxin A2



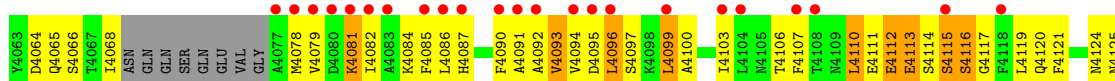


ASN

• Molecule 1: Voltatoxin A2



• Molecule 1: Voltatoxin 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 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.5 (28.54-3.20) 93.4 (28.54-3.20)	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)	Xtrriage
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	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 87.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage'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	0.66	0/1584	1.15	14/2150 (0.7%)
1	B	0.64	0/1584	1.03	6/2150 (0.3%)
1	C	0.65	1/1584 (0.1%)	0.98	7/2150 (0.3%)
1	D	0.57	0/1584	1.00	9/2150 (0.4%)
1	E	0.60	0/1522	1.12	14/2065 (0.7%)
All	All	0.63	1/7858 (0.0%)	1.06	50/10665 (0.5%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2018	ILE	CA-CB	-8.17	1.50	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ALA	N-CA-C	-9.38	100.42	113.37
1	D	3146	ALA	CA-C-N	9.22	128.90	118.85
1	D	3146	ALA	C-N-CA	9.22	128.90	118.85
1	E	4013	LEU	CA-C-N	8.79	128.81	119.76
1	E	4013	LEU	C-N-CA	8.79	128.81	119.76
1	A	13	LEU	CA-C-N	7.99	127.99	119.76
1	A	13	LEU	C-N-CA	7.99	127.99	119.76
1	E	4095	ASP	N-CA-C	7.51	120.68	107.61
1	D	3023	GLN	N-CA-C	-7.46	103.15	111.28
1	E	4021	SER	N-CA-C	-7.19	103.38	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	PHE	N-CA-C	-7.11	103.59	112.90
1	C	2086	LEU	N-CA-C	-6.98	103.67	111.28
1	D	3145	ASN	N-CA-C	-6.66	104.91	113.16
1	E	4126	VAL	N-CA-C	6.53	116.67	110.53
1	A	126	VAL	N-CA-C	6.36	117.71	111.67
1	D	3089	ALA	N-CA-C	6.27	117.78	111.07
1	E	4062	LYS	N-CA-C	6.22	117.86	108.46
1	C	2012	GLN	N-CA-C	-6.16	106.12	113.21
1	A	175	SER	N-CA-C	6.09	119.19	111.69
1	A	182	VAL	N-CA-C	6.08	117.05	108.17
1	E	4031	TYR	N-CA-C	6.02	119.14	108.24
1	C	2025	LEU	N-CA-C	-6.00	105.04	112.90
1	B	1095	ASP	N-CA-C	5.97	119.21	109.06
1	D	3108	THR	N-CA-C	-5.94	105.29	112.54
1	A	95	ASP	N-CA-C	5.89	118.08	108.55
1	A	21	SER	N-CA-C	-5.84	103.90	111.02
1	D	3011	ASP	N-CA-C	5.76	117.63	107.61
1	A	140	VAL	CA-C-N	5.74	125.71	120.03
1	A	140	VAL	C-N-CA	5.74	125.71	120.03
1	E	4099	LEU	N-CA-C	-5.72	106.94	114.04
1	A	8	GLN	CA-C-N	5.72	126.99	119.84
1	A	8	GLN	C-N-CA	5.72	126.99	119.84
1	E	4142	PHE	N-CA-C	-5.70	106.97	114.04
1	D	3154	VAL	N-CA-C	-5.57	99.05	107.73
1	C	2050	ILE	N-CA-C	-5.54	105.10	110.42
1	B	1182	VAL	N-CA-C	5.52	116.44	108.48
1	B	1149	TYR	N-CA-C	5.51	118.39	109.40
1	E	4116	SER	N-CA-C	5.44	117.55	110.53
1	B	1016	ASP	N-CA-C	5.42	117.18	111.28
1	E	4188	GLU	N-CA-C	5.40	119.03	109.96
1	A	149	TYR	N-CA-C	5.33	118.91	109.96
1	B	1135	ARG	N-CA-C	5.29	117.24	108.20
1	D	3078	MET	N-CA-C	-5.28	105.52	111.28
1	E	4091	ALA	N-CA-C	-5.28	106.09	113.37
1	B	1143	GLY	N-CA-C	-5.26	103.53	110.74
1	C	2008	GLN	CA-C-N	-5.17	114.66	120.14
1	C	2008	GLN	C-N-CA	-5.17	114.66	120.14
1	C	2191	VAL	N-CA-C	5.12	115.34	108.17
1	E	4100	ALA	N-CA-C	-5.09	106.17	112.38
1	E	4093	VAL	CB-CA-C	-5.08	107.40	111.71

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	169	0
1	B	1547	0	1515	157	0
1	C	1547	0	1515	193	0
1	D	1547	0	1515	185	0
1	E	1486	0	1461	158	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	843	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 55.

All (843) 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:E:4078:MET:HE1	1:E:4182:VAL:HG11	1.39	1.01
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:A:78:MET:HE1	1:A:182:VAL:HG11	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:C	1:A:92:ALA:H	1.77	0.90
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: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:C:2006:VAL:HG12	1:C:2135:ARG:HE	1.43	0.83
1:E:4078:MET:CE	1:E:4182:VAL:HG11	2.08	0.83
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:C:2026:LYS:O	1:C:2028:SER:N	2.17	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:6:VAL:HG23	1:A:7:PHE:CD2	2.22	0.74
1:A:120:GLN:HB3	1:A:133:GLU:HB3	1.68	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:A:78:MET:HE1	1:A:159:ILE:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:2071:GLN:O	1:C:2179:ASN:HA	1.89	0.72
1:C:2130:SER:OG	1:C:2163:ILE:HB	1.88	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:2037:ASP:C	1:C:2038:LYS:HD2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2074:GLU:N	1:C:2074:GLU:OE1	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:C:2128:LYS:HZ3	1:D:3098:LYS:HZ2	1.38	0.68
1:C:2090:PHE:O	1:C:2091:ALA:C	2.36	0.68
1:A:61:ASP:OD2	1:A:188:GLU:HG2	1.93	0.68
1:B:1159:ILE:N	1:B:1159:ILE:HD12	2.09	0.68
1:C:2128:LYS:NZ	1:D:3098:LYS:HZ2	1.92	0.68
1:B:1170:TRP:HE3	1:B:1170:TRP:N	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
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:B:1111:GLU:HB3	1:D:3069:ASN:CG	2.21	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: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:2091:ALA:C	1:C:2093:VAL:H	2.04	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:D:3103:ILE:O	1:D:3103:ILE:HG22	1.95	0.65
1:A:90:PHE:C	1:A:92:ALA:N	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3124:ASN:HB3	1:D:3127:LYS:HG2	1.80	0.64
1:B:1054:THR:O	1:B:1054:THR:HG23	1.96	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:E:4090:PHE:C	1:E:4092:ALA:H	2.03	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:B:1090:PHE:C	1:B:1092:ALA:H	2.04	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:D:3015:GLU:C	1:D:3017:LEU:H	2.06	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: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
1:E:4143:GLY:C	1:E:4145:ASN:H	2.07	0.63
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:B:1090:PHE:C	1:B:1092:ALA:N	2.55	0.62
1:C:2058:LEU:HD12	1:C:2195:PHE:CE1	2.34	0.62
1:C:2090:PHE:O	1:C:2092:ALA:N	2.32	0.62
1:B:1075:VAL:HG21	1:B:1173:THR:O	1.99	0.62
1:B:1090:PHE:O	1:B:1093:VAL:N	2.32	0.62
1:C:2090:PHE:C	1:C:2092:ALA:N	2.50	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:C:2013:LEU:HD23	1:C:2140:VAL:C	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:4006:VAL:CG1	1:E:4032:LEU:HD11	2.27	0.60
1:D:3007:PHE:CD1	1:D:3135:ARG:HB3	2.35	0.60
1:D:3098:LYS:HB2	1:D:3098:LYS:NZ	2.17	0.60
1:B:1184:ILE:HD13	1:B:1184:ILE:N	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:D:3078:MET:C	1:D:3080:ASP:H	2.10	0.60
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:1046:PHE:O	1:B:1047:LYS:C	2.46	0.59
1:B:1132:TRP:O	1:B:1158:LEU:HA	2.03	0.59
1:D:3090:PHE:C	1:D:3092:ALA:N	2.57	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:C:2128:LYS:HZ3	1:D:3098:LYS:NZ	2.01	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:B:1126:VAL:C	1:B:1128:LYS:H	2.12	0.58
1:C:2102:ILE:N	1:C:2102:ILE:HD12	2.18	0.58
1:E:4166:LYS:C	1:E:4168:GLY:N	2.60	0.58
1:A:96:LEU:O	1:A:99:LEU:HD21	2.02	0.58
1:B:1090:PHE:HD1	1:B:1188:GLU:CG	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1105:ASN:HD21	1:D:3183:GLN:HE22	1.49	0.58
1:C:2008:GLN:HE22	1:C:2102:ILE:HG21	1.69	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: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:A:99:LEU:HG	1:A:100:ALA:N	2.19	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:C:2173:THR:O	1:C:2174:SER:C	2.47	0.57
1:B:1093:VAL:HG22	1:B:1151:TYR:CG	2.40	0.57
1:B:1126:VAL:HG12	1:B:1127:LYS:N	2.19	0.57
1:E:4166:LYS:C	1:E:4168:GLY:H	2.10	0.57
1:B:1170:TRP:N	1:B:1170:TRP:CE3	2.72	0.57
1:B:1090:PHE:O	1:B:1092:ALA:N	2.38	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
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:E:4126:VAL:C	1:E:4128:LYS:H	2.13	0.57
1:C:2128:LYS:NZ	1:D:3098:LYS:NZ	2.52	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:D:3135:ARG:C	1:D:3136:VAL:HG22	2.30	0.56
1:E:4068:ILE:HD13	1:E:4081:LYS:HD2	1.86	0.56
1:E:4143:GLY:C	1:E:4145:ASN:N	2.63	0.56
1:B:1136:VAL:HG13	1:B:1136:VAL:O	2.06	0.56
1:D:3073:GLN:HG2	1:D:3180:PHE:HB2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:2099:LEU:C	1:C:2101:ALA:H	2.12	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:D:3094:VAL:HG11	1:D:3099:LEU:HD22	1.87	0.56
1:E:4187:LEU:C	1:E:4187:LEU:HD23	2.31	0.56
1:B:1035:GLU:HG3	1:B:1035:GLU:O	2.06	0.55
1:C:2073:GLN:O	1:C:2177:LYS:HA	2.06	0.55
1:B:1011:ASP:OD2	1:B:1011:ASP:C	2.50	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: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:E:4129:ASN:C	1:E:4129:ASN:OD1	2.49	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
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:C:2005:ASN:O	1:C:2117:GLY:C	2.49	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:C:2074:GLU:N	1:C:2074:GLU:CD	2.64	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:187:LEU:C	1:A:187:LEU:HD23	2.32	0.54
1:E:4050:ILE:HG21	1:E:4060:PHE:HB2	1.90	0.54
1:E:4112:GLU:O	1:E:4113:GLU:C	2.51	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:A:166:LYS:C	1:A:168:GLY:H	2.15	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:B:1075:VAL:O	1:B:1078:MET:HB3	2.07	0.54
1:B:1165:GLU:C	1:B:1167:THR:H	2.16	0.54
1:C:2099:LEU:C	1:C:2101:ALA:N	2.66	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:B:1161:ALA:C	1:B:1163:ILE:H	2.15	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:C:2155:THR:HG23	1:C:2186:ALA:HB2	1.90	0.53
1:C:2178:LYS:O	1:C:2180:PHE:HD2	1.90	0.53
1:D:3014:PRO:O	1:D:3015:GLU:C	2.51	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:B:1097:SER:C	1:B:1099:LEU:N	2.64	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:NZ	1:E:4081:LYS:HB2	2.24	0.53
1:B:1031:TYR:O	1:B:1042:ASP:HB3	2.08	0.53
1:B:1132:TRP:HE1	1:B:1169:TRP:CG	2.27	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:B:1036:GLN:C	1:B:1038:LYS:H	2.15	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:D:3007:PHE:O	1:D:3009:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:3090:PHE:O	1:D:3091:ALA:C	2.51	0.53
1:A:166:LYS:C	1:A:168:GLY:N	2.66	0.52
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:D:3027:PHE:HD1	1:D:3027:PHE:C	2.17	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:C:2014:PRO:O	1:C:2015:GLU:C	2.53	0.52
1:C:2137:LEU:C	1:C:2137:LEU:HD22	2.33	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:C:2018:ILE:O	1:C:2019:PRO:C	2.49	0.52
1:D:3087:HIS:CD2	1:D:3096:LEU:HB2	2.45	0.52
1:B:1098:LYS:O	1:B:1098:LYS:HD3	2.10	0.51
1:D:3027:PHE:C	1:D:3027:PHE:CD1	2.87	0.51
1:D:3083:ALA:HB1	1:D:3099:LEU:HD23	1.92	0.51
1:A:33:LYS:O	1:A:34:LEU:C	2.53	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:75:VAL:C	1:A:77:ALA:H	2.18	0.51
1:D:3055:GLY:C	1:D:3057:ASP:H	2.17	0.51
1:D:3134:TYR:C	1:D:3135:ARG:HD2	2.36	0.51
1:A:74:GLU:O	1:A:75:VAL:C	2.53	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
1:C:2087:HIS:HA	1:C:2094:VAL:HB	1.93	0.51
1:D:3104:LEU:C	1:D:3106:THR:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:3107:PHE:C	1:D:3110:LEU:HG	2.36	0.51
1:A:194:GLY:O	1:A:195:PHE:C	2.53	0.51
1:B:1015:GLU:O	1:B:1019:PRO:HD3	2.10	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:C:2038:LYS:HD2	1:C:2038:LYS:N	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:C:2132:TRP:HE1	1:C:2169:TRP:CG	2.30	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:D:3111:GLU:C	1:D:3113:GLU:N	2.68	0.50
1:D:3177:LYS:HB2	1:D:3177:LYS:HZ3	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
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:C:2036:GLN:C	1:C:2038:LYS:H	2.19	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: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:3032:LEU:CD1	1:D:3135:ARG:HH12	2.25	0.50
1:D:3079:VAL:HA	1:D:3082:ILE:CG2	2.42	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:4090:PHE:C	1:E:4092:ALA:N	2.67	0.50
1:B:1107:PHE:C	1:B:1109:ASN:H	2.20	0.49
1:E:4163:ILE:HG21	1:E:4169:TRP:CD1	2.46	0.49
1:C:2090:PHE:CD1	1:C:2188:GLU:HB2	2.47	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:E:4113:GLU:O	1:E:4114:SER:C	2.55	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:D:3090:PHE:C	1:D:3092:ALA:H	2.20	0.49
1:B:1071:GLN:O	1:B:1179:ASN:HA	2.13	0.49
1:C:2074:GLU:CD	1:C:2074:GLU:H	2.21	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:A:96:LEU:O	1:A:99:LEU:CD2	2.60	0.49
1:B:1093:VAL:HG21	1:B:1188:GLU:CD	2.38	0.49
1:B:1127:LYS:O	1:B:1127:LYS:HG3	2.12	0.49
1:E:4023:GLN:HG3	1:E:4196:LYS:HA	1.94	0.49
1:A:75:VAL:C	1:A:77:ALA:N	2.71	0.49
1:A:126:VAL:C	1:A:128:LYS:H	2.20	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:B:1086:LEU:C	1:B:1088:ASP:H	2.21	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:A:13:LEU:HD12	1:A:13:LEU:C	2.37	0.48
1:B:1030:LYS:O	1:B:1031:TYR:CD2	2.66	0.48
1:C:2091:ALA:C	1:C:2093:VAL:N	2.71	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:D:3015:GLU:C	1:D:3017:LEU:N	2.68	0.48
1:E:4046:PHE:CE2	1:E:4050:ILE:HD11	2.47	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:HD13	1:C:2137:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2032:LEU:HA	1:C:2042:ASP:N	2.22	0.48
1:E:4060:PHE:C	1:E:4060:PHE:CD2	2.91	0.48
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:3171:GLY:C	1:D:3172:LEU:HD12	2.38	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:150:PHE:CZ	1:A:191:VAL:HB	2.49	0.48
1:B:1166:LYS:O	1:B:1166:LYS:HG2	2.13	0.48
1:C:2041:PHE:HE1	1:C:2043:TRP:CE3	2.32	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:C:2029:GLY:C	1:C:2031:TYR:H	2.22	0.48
1:C:2092:ALA:O	1:C:2093:VAL:HB	2.12	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:46:PHE:CZ	1:A:50:ILE:HD11	2.49	0.47
1:A:58:LEU:HB2	1:A:195:PHE:CD1	2.48	0.47
1:A:60:PHE:C	1:A:60:PHE:CD2	2.92	0.47
1:B:1126:VAL:C	1:B:1128:LYS:N	2.70	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: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: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:2071:GLN:HE22	1:C:2073:GLN:CD	2.23	0.47
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: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:D:3124:ASN:C	1:D:3126:VAL:H	2.23	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:B:1163:ILE:HD11	1:B:1178:LYS:HE3	1.97	0.47
1:B:1173:THR:CG2	1:B:1174:SER:N	2.72	0.47
1:C:2112:GLU:H	1:C:2112:GLU:CD	2.22	0.47
1:E:4081:LYS:O	1:E:4084:LYS:HB3	2.14	0.47
1:C:2047:LYS:O	1:C:2049:ALA:N	2.48	0.47
1:A:38:LYS:HD3	1:A:122:ASN:OD1	2.14	0.47
1:A:126:VAL:C	1:A:128:LYS:N	2.71	0.47
1:B:1018:ILE:O	1:B:1019:PRO:C	2.57	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:C:2114:SER:C	1:C:2116:SER:H	2.23	0.47
1:A:43:TRP:HZ3	1:A:187:LEU:HB2	1.77	0.47
1:A:121:PHE:HB2	1:A:132:TRP:CH2	2.50	0.47
1:A:133:GLU:OE2	1:A:133:GLU:CA	2.62	0.47
1:A:143:GLY:C	1:A:145:ASN:H	2.22	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:A:87:HIS:ND1	1:A:87:HIS:C	2.74	0.46
1:C:2058:LEU:O	1:C:2059:SER:HB2	2.15	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:B:1058:LEU:C	1:B:1058:LEU:HD23	2.41	0.46
1:B:1068:ILE:HD12	1:B:1182:VAL:HB	1.97	0.46
1:C:2047:LYS:C	1:C:2049:ALA:H	2.23	0.46
1:E:4110:LEU:O	1:E:4111:GLU:C	2.57	0.46
1:E:4125:ASN:O	1:E:4128:LYS:NZ	2.45	0.46
1:A:34:LEU:O	1:A:35:GLU:HB2	2.15	0.46
1:C:2171:GLY:O	1:C:2172:LEU:C	2.58	0.46
1:D:3111:GLU:O	1:D:3113:GLU:N	2.48	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:HG3	1:D:3056:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4015:GLU:C	1:E:4017:LEU:H	2.23	0.46
1:A:110:LEU:O	1:A:111:GLU:C	2.57	0.46
1:A:129:ASN:OD1	1:A:129:ASN:C	2.58	0.46
1:C:2098:LYS:HE2	1:C:2102:ILE:HD11	1.97	0.46
1:D:3119:LEU:O	1:D:3132:TRP:HZ3	1.99	0.46
1:D:3121:PHE:HE1	1:D:3130:SER:HB3	1.80	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: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:3067:THR:HG22	1:D:3068:ILE:N	2.29	0.46
1:D:3118:PHE:O	1:D:3135:ARG:HD3	2.16	0.46
1:E:4043:TRP:CZ3	1:E:4187:LEU:HB2	2.51	0.46
1:E:4128:LYS:HG3	1:E:4164:GLU:OE1	2.15	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: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:E:4086:LEU:O	1:E:4087:HIS:C	2.57	0.46
1:E:4127:LYS:O	1:E:4128:LYS:C	2.58	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:3058:LEU:C	1:D:3058:LEU:HD23	2.41	0.46
1:D:3110:LEU:O	1:D:3113:GLU:C	2.58	0.46
1:A:18:ILE:HD12	1:D:3146:ALA:HB2	1.97	0.45
1:A:82:ILE:HG21	1:A:157:ILE:CD1	2.46	0.45
1:C:2090:PHE:C	1:C:2092:ALA:H	2.25	0.45
1:A:15:GLU:HA	1:A:18:ILE:HD12	1.97	0.45
1:C:2036:GLN:O	1:C:2036:GLN:HG3	2.16	0.45
1:C:2047:LYS:C	1:C:2049:ALA:N	2.75	0.45
1:E:4015:GLU:C	1:E:4017:LEU:N	2.72	0.45
1:A:36:GLN:HA	1:A:36:GLN:NE2	2.32	0.45
1:A:93:VAL:HG23	1:A:188:GLU:OE1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3132:TRP:HD1	1:D:3169:TRP:CD2	2.33	0.45
1:E:4114:SER:C	1:E:4116:SER:N	2.74	0.45
1:E:4178:LYS:HB3	1:E:4180:PHE:CZ	2.52	0.45
1:A:74:GLU:O	1:A:77:ALA:N	2.39	0.45
1:A:82:ILE:HD13	1:A:157:ILE:HD13	1.99	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:D:3128:LYS:C	1:D:3129:ASN:HD22	2.24	0.45
1:E:4034:LEU:HG	1:E:4035:GLU:N	2.31	0.45
1:A:63:TYR:O	1:A:64:ASP:HB2	2.16	0.45
1:A:132:TRP:O	1:A:158:LEU:HA	2.16	0.45
1:C:2043:TRP:O	1:C:2044:PRO:C	2.59	0.45
1:B:1165:GLU:C	1:B:1167:THR:N	2.74	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:O	1:C:2030:LYS:HG3	2.17	0.45
1:E:4015:GLU:O	1:E:4019:PRO:HD3	2.17	0.45
1:B:1074:GLU:O	1:B:1075:VAL:C	2.59	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: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:A:90:PHE:CE2	1:A:186:ALA:HB3	2.52	0.45
1:A:161:ALA:HB2	1:A:180:PHE:HD1	1.81	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:C:2165:GLU:C	1:C:2167:THR:H	2.25	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:4060:PHE:HA	1:E:4189:LEU:HD23	1.98	0.45
1:E:4126:VAL:C	1:E:4128:LYS:N	2.72	0.45
1:C:2096:LEU:HD22	1:C:2097:SER:H	1.76	0.44
1:D:3187:LEU:HD23	1:D:3187:LEU:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLN:HB2	1:A:38:LYS:HE2	1.99	0.44
1:B:1036:GLN:C	1:B:1038:LYS:N	2.75	0.44
1:C:2142:PHE:HZ	1:E:4022:ILE:CD1	2.27	0.44
1:D:3013:LEU:HG	1:D:3139:SER:O	2.17	0.44
1:D:3069:ASN:O	1:D:3071:GLN:HG2	2.18	0.44
1:A:74:GLU:O	1:A:77:ALA:CB	2.65	0.44
1:B:1155:THR:HB	1:B:1186:ALA:HB2	1.99	0.44
1:A:155:THR:HG22	1:A:156:THR:N	2.31	0.44
1:A:175:SER:O	1:A:176:THR:C	2.60	0.44
1:E:4162:ASP:CG	1:E:4179:ASN:HB2	2.43	0.44
1:A:46:PHE:O	1:A:46:PHE:CG	2.70	0.44
1:A:62:LYS:HG2	1:A:63:TYR:N	2.31	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:3032:LEU:HD23	1:D:3032:LEU:C	2.43	0.44
1:D:3062:LYS:HE3	1:D:3064:ASP:HB2	1.98	0.44
1:B:1111:GLU:HB3	1:D:3069:ASN:OD1	2.17	0.44
1:C:2128:LYS:O	1:C:2164:GLU:OE1	2.36	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: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:E:4175:SER:O	1:E:4176:THR:C	2.61	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:B:1044:PRO:O	1:B:1047:LYS:HB2	2.17	0.44
1:B:1147:PRO:C	1:B:1149:TYR:H	2.25	0.44
1:C:2023:GLN:C	1:C:2025:LEU:N	2.75	0.44
1:D:3015:GLU:HA	1:D:3018:ILE:CG1	2.47	0.43
1:B:1048:THR:O	1:B:1049:ALA:C	2.61	0.43
1:C:2057:ASP:O	1:C:2191:VAL:HA	2.19	0.43
1:A:73:GLN:HE21	1:A:180:PHE:HB2	1.82	0.43
1:C:2011:ASP:C	1:C:2013:LEU:H	2.24	0.43
1:C:2057:ASP:OD2	1:C:2057:ASP:N	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:36:GLN:HA	1:A:36:GLN:HE21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TRP:CH2	1:A:187:LEU:HB2	2.53	0.43
1:A:88:ASP:O	1:A:89:ALA:C	2.59	0.43
1:B:1042:ASP:O	1:B:1042:ASP:CG	2.62	0.43
1:D:3078:MET:C	1:D:3080:ASP:N	2.74	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:D:3036:GLN:C	1:D:3038:LYS:H	2.26	0.43
1:D:3194:GLY:O	1:D:3195:PHE:C	2.57	0.43
1:E:4024:VAL:HG21	1:E:4191:VAL:HG21	1.99	0.43
1:A:162:ASP:C	1:A:163:ILE:HD12	2.43	0.43
1:B:1097:SER:C	1:B:1099:LEU:H	2.27	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:4078:MET:HE3	1:E:4078:MET:HB2	1.74	0.43
1:A:53:TYR:CE2	1:A:58:LEU:HB3	2.53	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:3111:GLU:C	1:D:3113:GLU:H	2.27	0.43
1:D:3138:PHE:HB2	1:D:3153:LEU:HB2	2.00	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:E:4014:PRO:O	1:E:4015:GLU:C	2.60	0.43
1:B:1086:LEU:HB3	1:B:1094:VAL:HG21	2.01	0.43
1:C:2007:PHE:HD1	1:C:2135:ARG:C	2.27	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:40:TYR:CD1	1:A:133:GLU:HG2	2.54	0.42
1:A:107:PHE:CZ	1:A:159:ILE:HD13	2.54	0.42
1:A:161:ALA:O	1:A:163:ILE:N	2.52	0.42
1:B:1026:LYS:HG2	1:B:1026:LYS:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:VAL:HG11	1:B:1138:PHE:HE1	1.83	0.42
1:B:1132:TRP:C	1:B:1158:LEU:HD12	2.44	0.42
1:B:1134:TYR:HB3	1:B:1157:ILE:HB	2.01	0.42
1:B:1192:LYS:O	1:B:1193:LYS:C	2.62	0.42
1:C:2105:ASN:O	1:C:2106:THR:C	2.62	0.42
1:C:2119:LEU:HD23	1:C:2119:LEU:HA	1.80	0.42
1:D:3106:THR:O	1:D:3110:LEU:HD23	2.19	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: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:163:ILE:CG2	1:A:168:GLY:HA3	2.49	0.42
1:D:3110:LEU:O	1:D:3114:SER:N	2.52	0.42
1:E:4053:TYR:CE2	1:E:4055:GLY:HA3	2.54	0.42
1:A:79:VAL:C	1:A:81:LYS:N	2.77	0.42
1:B:1034:LEU:HD23	1:B:1039:ALA:HB2	2.01	0.42
1:B:1159:ILE:N	1:B:1159:ILE:CD1	2.80	0.42
1:C:2071:GLN:HE21	1:C:2071:GLN:CA	2.33	0.42
1:C:2136:VAL:HG12	1:C:2137:LEU:H	1.83	0.42
1:D:3050:ILE:HD11	1:D:3187:LEU:HD11	2.00	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:E:4058:LEU:CD2	1:E:4191:VAL:HG22	2.49	0.42
1:E:4090:PHE:CE2	1:E:4186:ALA:HB3	2.55	0.42
1:E:4096:LEU:HB3	1:E:4097:SER:H	1.49	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: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: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: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:A:24:VAL:CG2	1:A:191:VAL:HG21	2.49	0.42
1:A:143:GLY:C	1:A:145:ASN:N	2.78	0.42
1:B:1014:PRO:O	1:B:1015:GLU:C	2.63	0.42
1:C:2073:GLN:C	1:C:2177:LYS:HG3	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:4049:ALA:O	1:E:4050:ILE:C	2.62	0.42
1:A:106:THR:HG23	1:A:113:GLU:HG2	2.02	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: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:E:4114:SER:O	1:E:4115:SER:C	2.63	0.41
1:E:4124:ASN:O	1:E:4124:ASN:CG	2.63	0.41
1:A:99:LEU:C	1:A:101:ALA:N	2.77	0.41
1:A:107:PHE:HA	1:A:110:LEU:HD23	2.00	0.41
1:A:124:ASN:O	1:A:125:ASN:C	2.63	0.41
1:A:126:VAL:O	1:A:128:LYS:N	2.53	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
1:C:2187:LEU:HD23	1:C:2187:LEU:O	2.20	0.41
1:D:3121:PHE:CG	1:D:3122:ASN:N	2.88	0.41
1:B:1082:ILE:HG21	1:B:1157:ILE:HD13	2.03	0.41
1:C:2107:PHE:CE1	1:C:2159:ILE:HD13	2.56	0.41
1:C:2121:PHE:CG	1:C:2122:ASN:N	2.88	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:D:3164:GLU:O	1:D:3165:GLU:C	2.64	0.41
1:E:4068:ILE:O	1:E:4068:ILE:HG22	2.20	0.41
1:B:1121:PHE:CE1	1:B:1130:SER:HB2	2.55	0.41
1:E:4047:LYS:O	1:E:4048:THR:C	2.64	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:2071:GLN:HE21	1:C:2071:GLN:C	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3008:GLN:HE21	1:D:3008:GLN:HB3	1.71	0.41
1:D:3025:LEU:HD13	1:D:3137:LEU:HD12	2.02	0.41
1:D:3110:LEU:HD22	1:D:3119:LEU:HD13	2.03	0.41
1:B:1020:SER:O	1:B:1023:GLN:HB2	2.21	0.41
1:B:1027:PHE:O	1:B:1028:SER:C	2.63	0.41
1:B:1060:PHE:CE1	1:B:1062:LYS:C	2.99	0.41
1:D:3022:ILE:HG22	1:D:3022:ILE:O	2.20	0.41
1:D:3135:ARG:N	1:D:3135:ARG:CD	2.82	0.41
1:E:4120:GLN:HB3	1:E:4133:GLU:CB	2.46	0.41
1:A:132:TRP:HE1	1:A:169:TRP:CG	2.39	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:D:3032:LEU:HD11	1:D:3135:ARG:HH12	1.85	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:E:4033:LYS:O	1:E:4033:LYS:CG	2.69	0.41
1:E:4064:ASP:OD1	1:E:4065:GLN:N	2.54	0.41
1:A:98:LYS:HE2	1:C:2044:PRO:HG2	2.02	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: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: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:E:4043:TRP:HZ3	1:E:4187:LEU:CB	2.34	0.40
1:C:2041:PHE:HZ	1:C:2046:PHE:CG	2.39	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:3051:ASP:C	1:D:3053:TYR:H	2.29	0.40
1:D:3111:GLU:HG3	1:D:3170:TRP:HE1	1.85	0.40
1:E:4133:GLU:OE2	1:E:4133:GLU:CA	2.69	0.40
1:E:4166:LYS:O	1:E:4168:GLY:N	2.54	0.40
1:A:5:ASN:HD22	1:A:5:ASN:HA	1.56	0.40
1:A:60:PHE:CD1	1:A:187:LEU:HD21	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:21:SER:O	1:A:22:ILE:C	2.64	0.40
1:B:1070:GLN:HA	1:B:1180:PHE:O	2.22	0.40
1:B:1146:ALA:O	1:B:1149:TYR:N	2.43	0.40
1:B:1150:PHE:CZ	1:B:1191:VAL:HB	2.56	0.40
1:B:1184:ILE:O	1:B:1184:ILE:HG12	2.20	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:D:3166:LYS:C	1:D:3168:GLY:N	2.78	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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	192/199 (96%)	153 (80%)	29 (15%)	10 (5%)	1 12
1	B	192/199 (96%)	153 (80%)	26 (14%)	13 (7%)	1 7
1	C	192/199 (96%)	139 (72%)	29 (15%)	24 (12%)	0 1
1	D	192/199 (96%)	138 (72%)	35 (18%)	19 (10%)	0 2
1	E	182/199 (92%)	148 (81%)	30 (16%)	4 (2%)	5 29
All	All	950/995 (96%)	731 (77%)	149 (16%)	70 (7%)	1 6

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	B	1116	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/175 (98%)	150 (88%)	21 (12%)	4	22
1	B	171/175 (98%)	154 (90%)	17 (10%)	7	31
1	C	171/175 (98%)	153 (90%)	18 (10%)	6	28
1	D	171/175 (98%)	148 (86%)	23 (14%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	164/175 (94%)	150 (92%)	14 (8%)	10	37
All	All	848/875 (97%)	755 (89%)	93 (11%)	6	26

All (93) 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	69	ASN
1	A	81	LYS
1	A	95	ASP
1	A	110	LEU
1	A	113	GLU
1	A	125	ASN
1	A	128	LYS
1	A	133	GLU
1	A	154	VAL
1	A	159	ILE
1	A	160	THR
1	A	170	TRP
1	A	172	LEU
1	A	173	THR
1	A	183	GLN
1	B	1005	ASN
1	B	1006	VAL
1	B	1009	PRO
1	B	1075	VAL
1	B	1105	ASN
1	B	1116	SER
1	B	1123	THR
1	B	1133	GLU
1	B	1140	VAL
1	B	1155	THR
1	B	1159	ILE
1	B	1170	TRP
1	B	1173	THR
1	B	1184	ILE
1	B	1185	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1188	GLU
1	B	1189	LEU
1	C	2019	PRO
1	C	2048	THR
1	C	2071	GLN
1	C	2074	GLU
1	C	2096	LEU
1	C	2102	ILE
1	C	2105	ASN
1	C	2109	ASN
1	C	2112	GLU
1	C	2136	VAL
1	C	2137	LEU
1	C	2140	VAL
1	C	2152	SER
1	C	2167	THR
1	C	2170	TRP
1	C	2182	VAL
1	C	2185	ASP
1	C	2193	LYS
1	D	3011	ASP
1	D	3017	LEU
1	D	3019	PRO
1	D	3023	GLN
1	D	3025	LEU
1	D	3030	LYS
1	D	3047	LYS
1	D	3051	ASP
1	D	3079	VAL
1	D	3086	LEU
1	D	3096	LEU
1	D	3098	LYS
1	D	3107	PHE
1	D	3114	SER
1	D	3123	THR
1	D	3132	TRP
1	D	3136	VAL
1	D	3140	VAL
1	D	3155	THR
1	D	3177	LYS
1	D	3188	GLU
1	D	3189	LEU

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Mol	Chain	Res	Type
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	4081	LYS
1	E	4096	LEU
1	E	4110	LEU
1	E	4112	GLU
1	E	4113	GLU
1	E	4159	ILE
1	E	4170	TRP
1	E	4182	VAL
1	E	4183	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	8	GLN
1	A	12	GLN
1	A	36	GLN
1	A	52	ASN
1	A	65	GLN
1	A	105	ASN
1	A	122	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	1120	GLN
1	B	1125	ASN
1	B	1145	ASN
1	C	2008	GLN
1	C	2036	GLN
1	C	2052	ASN
1	C	2065	GLN
1	C	2070	GLN

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Mol	Chain	Res	Type
1	C	2071	GLN
1	C	2073	GLN
1	C	2109	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	3145	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 [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.36	1 (0%) 87 76	22, 56, 89, 108	0
1	B	194/199 (97%)	-0.25	2 (1%) 79 63	29, 59, 96, 126	0
1	C	194/199 (97%)	-0.21	0 100 100	22, 66, 103, 116	0
1	D	194/199 (97%)	0.03	3 (1%) 72 52	23, 84, 134, 155	0
1	E	186/199 (93%)	1.47	46 (24%) 2 2	70, 149, 185, 191	0
All	All	962/995 (96%)	0.12	52 (5%) 31 20	22, 71, 173, 191	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4094	VAL	6.3
1	E	4107	PHE	5.8
1	E	4039	ALA	5.3
1	E	4027	PHE	4.9
1	E	4176	THR	4.5
1	E	4081	LYS	4.5
1	E	4086	LEU	4.3
1	E	4082	ILE	4.2
1	E	4096	LEU	3.4
1	E	4172	LEU	3.4
1	E	4104	LEU	3.4
1	E	4083	ALA	3.3
1	E	4103	ILE	3.3
1	E	4137	LEU	3.2
1	E	4091	ALA	3.1
1	E	4078	MET	3.0
1	E	4034	LEU	2.9
1	E	4099	LEU	2.9
1	E	4028	SER	2.8
1	D	3091	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	4115	SER	2.7
1	E	4007	PHE	2.6
1	B	1092	ALA	2.6
1	E	4077	ALA	2.6
1	E	4134	TYR	2.6
1	E	4079	VAL	2.6
1	E	4092	ALA	2.5
1	E	4182	VAL	2.5
1	E	4138	PHE	2.5
1	E	4162	ASP	2.5
1	E	4174	SER	2.4
1	E	4159	ILE	2.4
1	E	4129	ASN	2.4
1	E	4133	GLU	2.3
1	E	4085	PHE	2.2
1	E	4108	THR	2.2
1	E	4187	LEU	2.2
1	D	3107	PHE	2.2
1	E	4087	HIS	2.2
1	E	4095	ASP	2.1
1	A	92	ALA	2.1
1	E	4090	PHE	2.1
1	E	4175	SER	2.1
1	D	3050	ILE	2.1
1	E	4135	ARG	2.0
1	E	4080	ASP	2.0
1	E	4156	THR	2.0
1	E	4046	PHE	2.0
1	B	1091	ALA	2.0
1	E	4031	TYR	2.0
1	E	4118	PHE	2.0
1	E	4024	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.