



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2018 – 10:42 PM EST

PDB ID : 1WE0
Title : Crystal structure of peroxiredoxin (AhpC) from *Amphibacillus xylanus*
Authors : Kitano, K.; Kita, A.; Hakoshima, T.; Niimura, Y.; Miki, K.
Deposited on : 2004-05-21
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

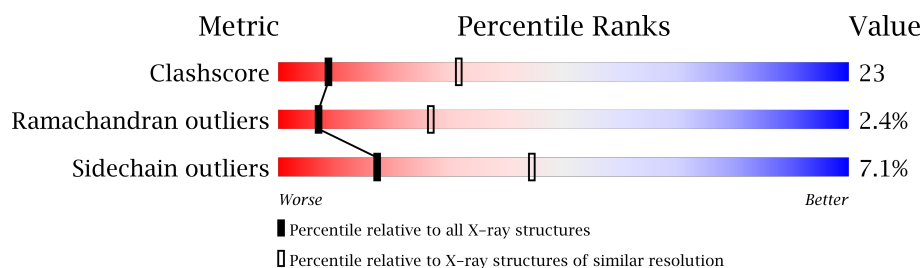
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)




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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	187	
1	B	187	
1	C	187	
1	D	187	
1	E	187	
1	F	187	
1	G	187	

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Mol	Chain	Length	Quality of chain
1	H	187	 47% 36% 5% 11%
1	I	187	 56% 29% • 11%
1	J	187	 50% 33% 5% 11%

2 Entry composition

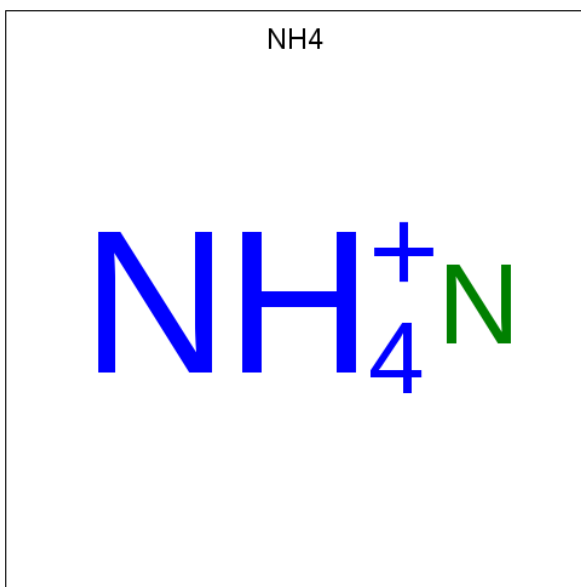
There are 2 unique types of molecules in this entry. The entry contains 12982 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 alkyl hydroperoxide reductase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	B	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	C	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	D	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	E	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	F	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	G	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	H	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	I	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			
1	J	166	Total	C	N	O	S	0	0	0
			1298	826	211	258	3			

- Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total	N	0	0
			1	1		
2	J	1	Total	N	0	0
			1	1		

Note EDS was not executed.

- Chain A: 48% 38% 11%

Amino Acid	Count
GLU	192
GLY	E93
GLY	Y94
GLY	I95
GLU	M96
THR	I97
LEU	G98
LYS	D99
PRO	P100
SER	S101
LEU	Q102
ASP	T103
ILE	I104
VAL	Q107
GLY	Q107
LYS	V110
ILE	L111
LYS	N112
LYS	T115
LEU	D119
LEU	R120
GLY	G121
LEU	T122
LYS	D126
GLY	A138
GLY	D139
GLY	G140
LYS	R143
GLY	S146
GLY	T147
GLY	L148
GLY	I149
GLY	N150
GLY	K151
GLY	V152
GLY	K153
GLY	A154
GLY	A155
GLY	Q156
GLY	Y157
GLY	V158
GLY	R159
GLY	E160
GLY	N161
GLY	P162
GLY	G163
GLY	E164
GLY	V165
GLY	C166
PRO	PRQ
GLY	ALQ
LYS	LYS
THR	TRD

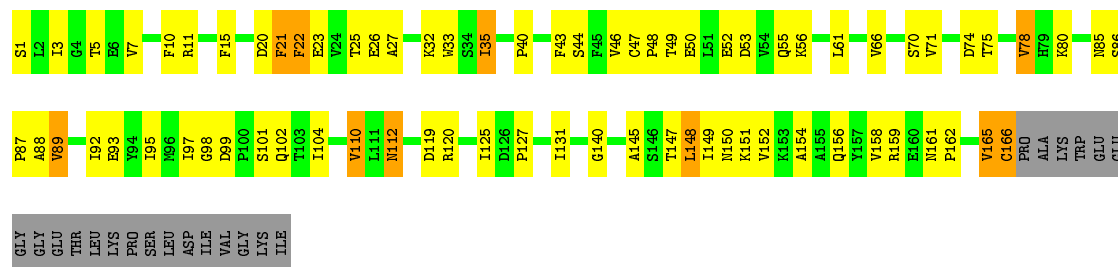
- Chain B:
-
- | Amino Acid | Count |
|------------|-------|
| S1 | 1 |
| L2 | 1 |
| I3 | 1 |
| G4 | 1 |
| T5 | 1 |
| E6 | 1 |
| V7 | 1 |
| R11 | 1 |
| D20 | 1 |
| F21 | 1 |
| F22 | 1 |
| E23 | 1 |
| V24 | 1 |
| T25 | 1 |
| E26 | 1 |
| A27 | 1 |
| D28 | 1 |
| L29 | 1 |
| K32 | 1 |
| K33 | 1 |
| S34 | 1 |
| I35 | 1 |
| V36 | 1 |
| V37 | 1 |
| F38 | 1 |
| Y39 | 1 |
| P40 | 1 |
| A41 | 1 |
| S44 | 1 |
| F45 | 1 |
| V46 | 1 |
| C47 | 1 |
| P48 | 1 |
| T49 | 1 |
| E50 | 1 |
| L51 | 1 |
| E60 | 1 |
| L64 | 1 |
| G85 | 1 |
| V66 | 1 |
| E67 | 1 |
| V68 | 1 |
| V71 | 1 |
| T75 | 1 |
| H76 | 1 |
| F77 | 1 |
| V78 | 1 |
| N85 | 1 |
| S86 | 1 |
| P87 | 1 |
| A88 | 1 |
| V89 | 1 |
| I92 | 1 |
| E93 | 1 |
| Y94 | 1 |
| I95 | 1 |
| P96 | 1 |
| I97 | 1 |
| G98 | 1 |
| D99 | 1 |
| P100 | 1 |
| S101 | 1 |
| A102 | 1 |
| T103 | 1 |
| I104 | 1 |
| S105 | 1 |
| R106 | 1 |
| Q107 | 1 |
| V110 | 1 |
| L111 | 1 |
| N112 | 1 |
| D119 | 1 |
| R120 | 1 |
| I125 | 1 |
| D126 | 1 |
| P127 | 1 |
| Q132 | 1 |
| I136 | 1 |
| G140 | 1 |
| A145 | 1 |
| S146 | 1 |
| T147 | 1 |
| L148 | 1 |
| I149 | 1 |
| N150 | 1 |
| K151 | 1 |
| V152 | 1 |
| K153 | 1 |
| A154 | 1 |
| K155 | 1 |
| Q156 | 1 |
| Y157 | 1 |
| V158 | 1 |
| R159 | 1 |
| E160 | 1 |
| L161 | 1 |
| P162 | 1 |
| V165 | 1 |
| C166 | 1 |
| P169 | 1 |
| A170 | 1 |
| V171 | 1 |

- Chain C: 55% 27% 7% 11%
- | Residue | Category |
|---------|----------|
| S1 | Green |
| L2 | Green |
| I3 | Green |
| F10 | Yellow |
| Q16 | Yellow |
| K19 | Orange |
| D20 | Orange |
| D21 | Orange |
| F22 | Orange |
| E26 | Yellow |
| A27 | Yellow |
| D28 | Yellow |
| L29 | Yellow |
| W33 | Yellow |
| S34 | Green |
| I35 | Orange |
| V36 | Orange |
| V37 | Yellow |
| F38 | Green |
| Y39 | Yellow |
| P40 | Yellow |
| C47 | Yellow |
| P48 | Yellow |
| T49 | Yellow |
| E50 | Yellow |
| L51 | Orange |
| E52 | Green |
| D53 | Yellow |
| V54 | Green |
| Q55 | Yellow |
| R56 | Yellow |
| V66 | Yellow |
| V71 | Yellow |
| S72 | Orange |
| T73 | Yellow |
| D74 | Green |
| T75 | Yellow |
| V78 | Orange |
| N85 | Yellow |
| S86 | Yellow |
| P87 | Yellow |
| A88 | Yellow |
| V89 | Yellow |
| I92 | Yellow |
| E93 | Yellow |
| Y94 | Yellow |
| I95 | Yellow |
| N96 | Green |
| I97 | Yellow |
| G98 | Green |
| D99 | Yellow |
| P100 | Yellow |
| S101 | Yellow |
| Q102 | Orange |
| T103 | Orange |
| I104 | Orange |
| V110 | Yellow |
| L111 | Yellow |
| N112 | Orange |
| T115 | Yellow |
| R120 | Yellow |
| P127 | Yellow |
| G140 | Yellow |
| I141 | Yellow |
| D144 | Yellow |
| A145 | Yellow |
| S146 | Yellow |
| T147 | Green |
| L148 | Orange |
| I149 | Yellow |
| K153 | Yellow |
| Q156 | Yellow |
| Y157 | Yellow |
| V158 | Yellow |
| R159 | Yellow |
| E160 | Green |
| N161 | Yellow |
| P162 | Yellow |
| G163 | Yellow |
| E164 | Yellow |
| V165 | Orange |
| C166 | Orange |
| P169 | Orange |
| A174 | Yellow |
| L175 | Yellow |
| T176 | Yellow |
| T177 | Yellow |
| GLU | Yellow |
| GLU | Yellow |
| GLY | Yellow |
| GLY | Yellow |
| GLU | Yellow |
| THR | Yellow |
| LEU | Yellow |
| LYS | Yellow |
| PRO | Yellow |
| SER | Yellow |
| LEU | Yellow |
| ASP | Yellow |
| ILE | Yellow |
| VAL | Yellow |
| GLY | Yellow |
- LYS

ILE

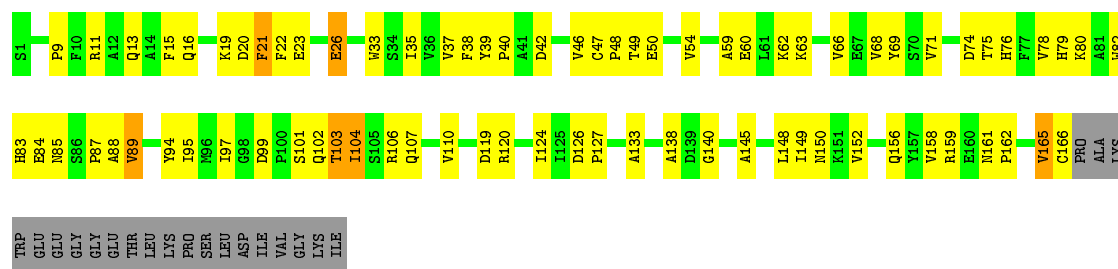
- Molecule 1: alkyl hydroperoxide reductase C

Chain D:  49% 34% 5% 11%



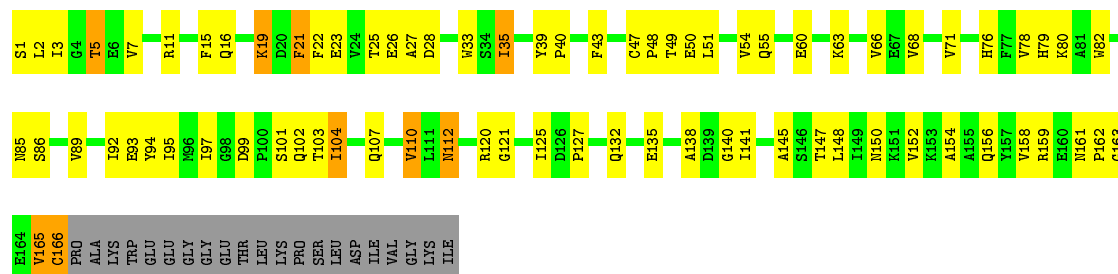
- Molecule 1: alkyl hydroperoxide reductase C

Chain E: 48% 37% 1% 11%



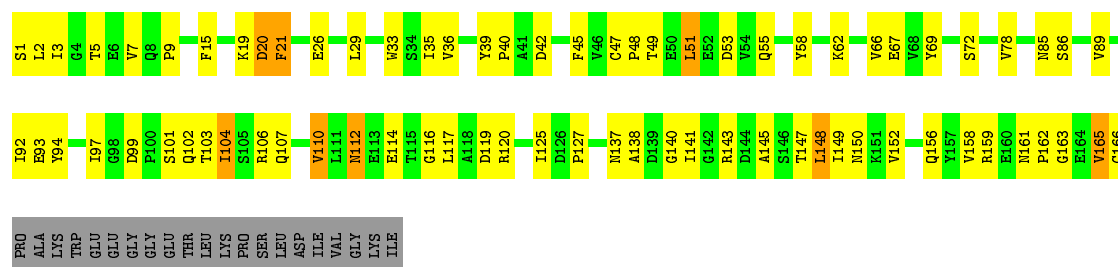
- Molecule 1: alkyl hydroperoxide reductase C

Chain F: 48% 36% 5% 11%



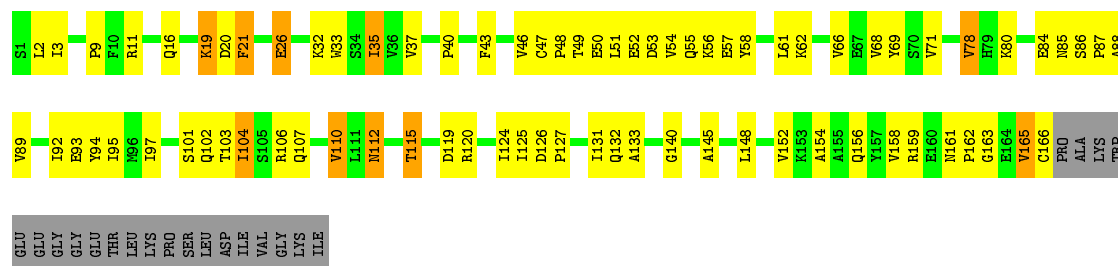
- Molecule 1: alkyl hydroperoxide reductase C

Chain G:  49% 35% 1% 15%



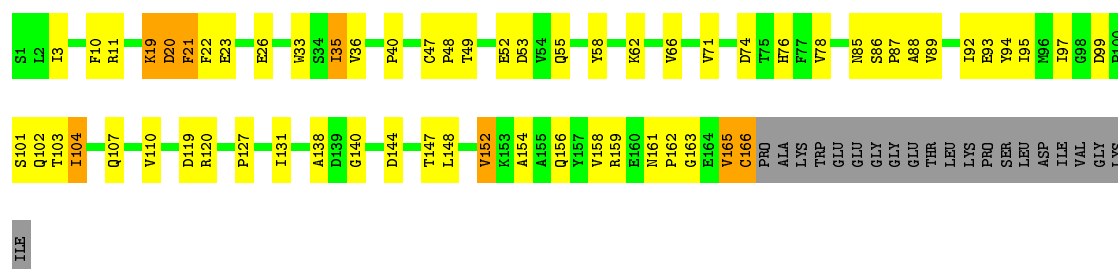
- Molecule 1: alkyl hydroperoxide reductase C

Chain H: 



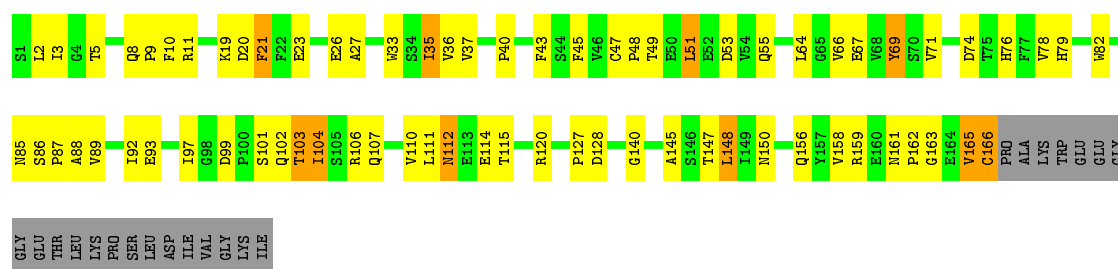
- Molecule 1: alkyl hydroperoxide reductase C

Chain I: 



- Molecule 1: alkyl hydroperoxide reductase C

Chain J: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.22Å 79.32Å 104.45Å 77.22° 82.33° 80.08°	Depositor
Resolution (Å)	50.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12982	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH4

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	0.44	0/1326	0.62	0/1800
1	B	0.42	0/1326	0.59	0/1800
1	C	0.44	0/1326	0.60	0/1800
1	D	0.39	0/1326	0.59	0/1800
1	E	0.37	0/1326	0.58	0/1800
1	F	0.42	0/1326	0.63	0/1800
1	G	0.41	0/1326	0.62	0/1800
1	H	0.41	0/1326	0.59	0/1800
1	I	0.41	0/1326	0.60	0/1800
1	J	0.45	0/1326	0.61	0/1800
All	All	0.42	0/13260	0.60	0/18000

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1298	0	1252	62	0
1	B	1298	0	1252	59	0
1	C	1298	0	1252	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1298	0	1252	69	0
1	E	1298	0	1252	55	0
1	F	1298	0	1252	66	0
1	G	1298	0	1252	61	0
1	H	1298	0	1252	73	0
1	I	1298	0	1252	57	0
1	J	1298	0	1252	68	0
2	F	1	0	0	0	0
2	J	1	0	0	0	0
All	All	12982	0	12520	576	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 23.

All (576) 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:A:85:ASN:ND2	1:J:85:ASN:HD22	1.53	1.06
1:B:85:ASN:HD22	1:C:85:ASN:HD22	1.12	0.96
1:D:85:ASN:HD22	1:E:85:ASN:ND2	1.63	0.96
1:A:85:ASN:HD22	1:J:85:ASN:HD22	1.03	0.94
1:H:85:ASN:HD22	1:I:85:ASN:HD22	1.13	0.92
1:J:106:ARG:HB2	1:J:106:ARG:HH11	1.34	0.92
1:H:85:ASN:HD22	1:I:85:ASN:ND2	1.69	0.89
1:E:103:THR:O	1:E:107:GLN:HG3	1.73	0.88
1:F:141:ILE:HD12	1:F:141:ILE:H	1.40	0.86
1:D:85:ASN:HD22	1:E:85:ASN:HD22	1.21	0.86
1:D:71:VAL:HG11	1:D:104:ILE:HD11	1.58	0.85
1:G:112:ASN:C	1:G:112:ASN:HD22	1.80	0.85
1:F:112:ASN:HD22	1:F:112:ASN:C	1.81	0.83
1:B:103:THR:O	1:B:107:GLN:HG3	1.82	0.80
1:C:140:GLY:HA3	1:D:158:VAL:HG21	1.62	0.80
1:J:106:ARG:NH1	1:J:106:ARG:HB2	1.96	0.80
1:I:148:LEU:O	1:I:152:VAL:HG12	1.81	0.79
1:I:140:GLY:HA3	1:J:158:VAL:HG21	1.66	0.78
1:F:1:SER:OG	1:F:3:ILE:HG22	1.84	0.78
1:B:85:ASN:ND2	1:C:85:ASN:HD22	1.82	0.77
1:I:158:VAL:HG21	1:J:140:GLY:HA3	1.66	0.77
1:E:11:ARG:HD2	1:E:23:GLU:CD	2.07	0.75
1:E:99:ASP:CG	1:E:104:ILE:HG23	2.08	0.74
1:E:83:HIS:HA	1:E:89:VAL:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:VAL:HG22	1:A:119:ASP:HB2	1.70	0.74
1:F:2:LEU:O	1:F:5:THR:HG23	1.86	0.74
1:H:52:GLU:HG3	1:H:56:LYS:HZ2	1.54	0.73
1:A:11:ARG:HD2	1:A:23:GLU:OE1	1.89	0.73
1:H:85:ASN:ND2	1:I:85:ASN:HD22	1.86	0.73
1:C:158:VAL:HG21	1:D:140:GLY:HA3	1.71	0.72
1:J:103:THR:O	1:J:107:GLN:HG3	1.88	0.72
1:C:112:ASN:C	1:C:112:ASN:HD22	1.93	0.72
1:H:85:ASN:ND2	1:I:85:ASN:ND2	2.38	0.71
1:H:52:GLU:HG3	1:H:56:LYS:NZ	2.06	0.71
1:A:37:VAL:HG12	1:A:122:THR:HG23	1.73	0.71
1:F:103:THR:O	1:F:107:GLN:HG3	1.90	0.71
1:A:74:ASP:HB3	1:A:78:VAL:HG11	1.72	0.70
1:I:156:GLN:O	1:I:159:ARG:HB3	1.91	0.70
1:D:61:LEU:HD22	1:D:66:VAL:HG11	1.73	0.70
1:D:71:VAL:CG1	1:D:104:ILE:HD11	2.21	0.70
1:J:99:ASP:CG	1:J:104:ILE:HG23	2.11	0.69
1:B:110:VAL:HG22	1:B:119:ASP:HB2	1.73	0.69
1:J:147:THR:HA	1:J:150:ASN:HD22	1.58	0.69
1:H:103:THR:O	1:H:107:GLN:HG3	1.93	0.69
1:A:148:LEU:O	1:A:152:VAL:HG13	1.93	0.68
1:A:85:ASN:HD22	1:J:85:ASN:ND2	1.87	0.68
1:D:85:ASN:ND2	1:E:85:ASN:ND2	2.38	0.68
1:G:66:VAL:HG21	1:G:152:VAL:HG21	1.75	0.68
1:J:106:ARG:CB	1:J:106:ARG:HH11	2.05	0.68
1:C:99:ASP:CG	1:C:104:ILE:HG23	2.15	0.67
1:D:53:ASP:HA	1:D:56:LYS:HE2	1.76	0.67
1:A:74:ASP:HB3	1:A:78:VAL:CG1	2.25	0.66
1:C:19:LYS:H	1:C:19:LYS:HD2	1.60	0.66
1:I:99:ASP:CG	1:I:104:ILE:HG23	2.14	0.66
1:D:85:ASN:ND2	1:E:85:ASN:HD22	1.93	0.66
1:J:87:PRO:HG2	1:J:88:ALA:H	1.61	0.66
1:J:112:ASN:HD21	1:J:114:GLU:HG3	1.60	0.66
1:F:120:ARG:HG2	1:F:120:ARG:HH11	1.60	0.66
1:H:57:GLU:O	1:H:61:LEU:HD12	1.96	0.66
1:G:112:ASN:HD21	1:G:114:GLU:HG2	1.60	0.65
1:B:11:ARG:HD2	1:B:23:GLU:OE1	1.95	0.65
1:I:87:PRO:HG2	1:I:88:ALA:H	1.61	0.65
1:D:156:GLN:O	1:D:159:ARG:HB3	1.97	0.65
1:F:66:VAL:HG21	1:F:152:VAL:HG21	1.77	0.65
1:D:112:ASN:C	1:D:112:ASN:HD22	1.98	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLN:O	1:B:159:ARG:HB3	1.98	0.64
1:A:154:ALA:O	1:A:158:VAL:HG23	1.98	0.64
1:C:165:VAL:O	1:C:166:CYS:HB2	1.98	0.64
1:H:112:ASN:OD1	1:H:115:THR:HG23	1.98	0.64
1:F:7:VAL:HG21	1:F:125:ILE:HD13	1.79	0.64
1:A:99:ASP:CG	1:A:104:ILE:HG23	2.17	0.63
1:B:154:ALA:O	1:B:158:VAL:HG23	1.98	0.63
1:I:71:VAL:HG22	1:I:97:ILE:HB	1.81	0.63
1:J:156:GLN:O	1:J:159:ARG:HB3	1.99	0.63
1:B:99:ASP:CG	1:B:104:ILE:HG23	2.19	0.63
1:I:120:ARG:HH11	1:I:120:ARG:HG2	1.62	0.63
1:G:1:SER:OG	1:G:3:ILE:HG22	1.99	0.62
1:H:53:ASP:HA	1:H:56:LYS:HZ3	1.64	0.62
1:H:55:GLN:OE1	1:H:92:ILE:HA	1.99	0.62
1:G:161:ASN:N	1:G:162:PRO:HD3	2.14	0.62
1:I:144:ASP:OD2	1:I:147:THR:HG23	1.99	0.62
1:A:103:THR:O	1:A:107:GLN:HG3	2.00	0.62
1:A:85:ASN:ND2	1:J:85:ASN:ND2	2.37	0.62
1:C:73:THR:HG22	1:C:99:ASP:O	2.00	0.62
1:E:110:VAL:HG22	1:E:119:ASP:HB2	1.82	0.62
1:G:140:GLY:HA3	1:H:158:VAL:HG21	1.80	0.62
1:A:1:SER:OG	1:A:3:ILE:HG22	1.98	0.62
1:F:161:ASN:N	1:F:162:PRO:HD3	2.14	0.62
1:B:2:LEU:O	1:B:5:THR:HG23	1.99	0.61
1:E:156:GLN:O	1:E:159:ARG:HB3	2.00	0.61
1:B:25:THR:C	1:B:27:ALA:H	2.04	0.61
1:E:138:ALA:HB2	1:F:3:ILE:HD11	1.82	0.61
1:G:110:VAL:HG22	1:G:119:ASP:HB2	1.82	0.61
1:E:74:ASP:HB3	1:E:78:VAL:CG1	2.30	0.61
1:H:145:ALA:HA	1:H:148:LEU:HD23	1.81	0.61
1:A:149:ILE:O	1:A:153:LYS:HG3	2.00	0.61
1:D:149:ILE:HG13	1:D:150:ASN:N	2.14	0.61
1:J:26:GLU:HG2	1:J:27:ALA:N	2.16	0.61
1:A:64:LEU:HD22	1:A:156:GLN:HE22	1.65	0.60
1:D:33:TRP:O	1:D:66:VAL:HA	2.01	0.60
1:A:79:HIS:ND1	1:A:96:MET:HB3	2.16	0.60
1:F:141:ILE:N	1:F:141:ILE:HD12	2.13	0.60
1:J:120:ARG:HG2	1:J:120:ARG:HH11	1.67	0.60
1:F:71:VAL:HG22	1:F:97:ILE:HB	1.84	0.60
1:F:120:ARG:HG2	1:F:120:ARG:NH1	2.16	0.60
1:G:99:ASP:CG	1:G:104:ILE:HG23	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:ASN:C	1:H:112:ASN:HD22	2.04	0.60
1:B:85:ASN:HD22	1:C:85:ASN:ND2	1.92	0.60
1:C:156:GLN:O	1:C:159:ARG:HB3	2.01	0.60
1:H:156:GLN:O	1:H:159:ARG:HB3	2.01	0.60
1:I:33:TRP:O	1:I:66:VAL:HA	2.01	0.60
1:H:33:TRP:O	1:H:66:VAL:HA	2.02	0.60
1:B:33:TRP:O	1:B:66:VAL:HA	2.02	0.59
1:G:145:ALA:O	1:G:148:LEU:HB2	2.01	0.59
1:B:60:GLU:O	1:B:64:LEU:HD12	2.03	0.59
1:F:112:ASN:C	1:F:112:ASN:ND2	2.54	0.59
1:A:161:ASN:N	1:A:162:PRO:HD3	2.17	0.59
1:F:147:THR:HA	1:F:150:ASN:HD22	1.67	0.59
1:G:158:VAL:HG21	1:H:140:GLY:HA3	1.84	0.59
1:C:33:TRP:O	1:C:66:VAL:HA	2.02	0.59
1:D:99:ASP:CG	1:D:104:ILE:HG12	2.22	0.59
1:E:158:VAL:HG21	1:F:140:GLY:HA3	1.84	0.59
1:H:71:VAL:HG22	1:H:97:ILE:HB	1.85	0.59
1:J:147:THR:HA	1:J:150:ASN:ND2	2.18	0.59
1:F:33:TRP:O	1:F:66:VAL:HA	2.01	0.59
1:I:120:ARG:HG2	1:I:120:ARG:NH1	2.18	0.59
1:E:33:TRP:O	1:E:66:VAL:HA	2.02	0.59
1:J:120:ARG:HG2	1:J:120:ARG:NH1	2.16	0.59
1:J:161:ASN:N	1:J:162:PRO:HD3	2.18	0.59
1:H:58:TYR:CZ	1:H:62:LYS:HE2	2.38	0.58
1:I:22:PHE:HZ	1:I:95:ILE:HD12	1.68	0.58
1:D:1:SER:OG	1:D:3:ILE:HG22	2.03	0.58
1:B:35:ILE:CD1	1:B:148:LEU:HG	2.33	0.58
1:E:74:ASP:HB3	1:E:78:VAL:HG11	1.83	0.58
1:E:161:ASN:N	1:E:162:PRO:HD3	2.18	0.58
1:G:33:TRP:O	1:G:66:VAL:HA	2.03	0.58
1:H:33:TRP:CE2	1:H:127:PRO:HD3	2.39	0.58
1:D:161:ASN:N	1:D:162:PRO:HD3	2.18	0.58
1:H:53:ASP:HA	1:H:56:LYS:CD	2.34	0.58
1:H:69:TYR:CE1	1:H:95:ILE:HG13	2.39	0.58
1:F:85:ASN:ND2	1:G:85:ASN:HB3	2.19	0.58
1:J:55:GLN:OE1	1:J:93:GLU:N	2.35	0.58
1:B:161:ASN:N	1:B:162:PRO:HD3	2.18	0.57
1:E:83:HIS:HA	1:E:89:VAL:CG2	2.33	0.57
1:D:11:ARG:HD2	1:D:23:GLU:CD	2.25	0.57
1:F:51:LEU:HB3	1:F:92:ILE:HD11	1.87	0.57
1:A:22:PHE:HZ	1:A:95:ILE:HD12	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:SER:OG	1:B:3:ILE:HG22	2.05	0.57
1:D:7:VAL:HG21	1:D:125:ILE:HD13	1.85	0.57
1:F:141:ILE:CD1	1:F:141:ILE:H	2.16	0.57
1:H:148:LEU:O	1:H:152:VAL:HG13	2.05	0.57
1:G:120:ARG:HH11	1:G:120:ARG:HG2	1.69	0.57
1:C:161:ASN:N	1:C:162:PRO:HD3	2.18	0.57
1:A:33:TRP:O	1:A:66:VAL:HA	2.05	0.57
1:C:22:PHE:HZ	1:C:95:ILE:HD12	1.70	0.57
1:F:55:GLN:OE1	1:F:93:GLU:N	2.35	0.56
1:F:55:GLN:OE1	1:F:92:ILE:HA	2.04	0.56
1:E:22:PHE:HZ	1:E:95:ILE:HD12	1.70	0.56
1:I:33:TRP:CE2	1:I:127:PRO:HD3	2.40	0.56
1:C:33:TRP:CE2	1:C:127:PRO:HD3	2.41	0.56
1:H:154:ALA:O	1:H:158:VAL:HG23	2.06	0.56
1:H:52:GLU:C	1:H:56:LYS:HZ2	2.08	0.56
1:G:2:LEU:O	1:G:5:THR:HG23	2.06	0.56
1:H:69:TYR:CD1	1:H:95:ILE:HB	2.40	0.56
1:J:89:VAL:HG23	1:J:92:ILE:HD12	1.87	0.56
1:I:35:ILE:O	1:I:35:ILE:HG12	2.06	0.56
1:J:99:ASP:OD1	1:J:104:ILE:HG23	2.06	0.56
1:B:75:THR:O	1:B:78:VAL:HG13	2.05	0.56
1:C:141:ILE:HD12	1:C:141:ILE:H	1.71	0.56
1:H:112:ASN:CG	1:H:115:THR:HG23	2.26	0.56
1:H:46:VAL:HG21	1:H:120:ARG:NH2	2.20	0.56
1:I:103:THR:O	1:I:107:GLN:HG3	2.06	0.56
1:C:101:SER:OG	1:C:103:THR:HG23	2.07	0.55
1:D:89:VAL:HG23	1:D:92:ILE:HD12	1.87	0.55
1:E:50:GLU:O	1:E:54:VAL:HG23	2.06	0.55
1:F:101:SER:O	1:F:102:GLN:HB2	2.07	0.55
1:H:52:GLU:O	1:H:56:LYS:HD2	2.06	0.55
1:B:51:LEU:HB3	1:B:92:ILE:HD11	1.89	0.55
1:F:2:LEU:C	1:F:5:THR:HG23	2.27	0.55
1:C:120:ARG:HG2	1:C:120:ARG:NH1	2.22	0.55
1:B:87:PRO:HG2	1:B:88:ALA:H	1.72	0.55
1:G:9:PRO:HA	1:G:26:GLU:OE1	2.06	0.55
1:H:112:ASN:OD1	1:H:115:THR:CG2	2.55	0.55
1:H:55:GLN:OE1	1:H:93:GLU:N	2.39	0.55
1:C:112:ASN:ND2	1:C:112:ASN:C	2.60	0.54
1:F:85:ASN:ND2	1:G:85:ASN:HD22	2.05	0.54
1:E:75:THR:O	1:E:78:VAL:HG12	2.07	0.54
1:J:86:SER:HB3	1:J:89:VAL:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:86:SER:OG	1:J:89:VAL:HG12	2.08	0.54
1:B:99:ASP:OD1	1:B:104:ILE:HG23	2.07	0.54
1:D:33:TRP:CD2	1:D:127:PRO:HD3	2.43	0.54
1:F:148:LEU:O	1:F:152:VAL:HG12	2.07	0.54
1:D:112:ASN:C	1:D:112:ASN:ND2	2.60	0.54
1:J:33:TRP:O	1:J:66:VAL:HA	2.07	0.54
1:C:87:PRO:HG2	1:C:88:ALA:H	1.72	0.54
1:H:124:ILE:HB	1:H:133:ALA:HB3	1.90	0.54
1:B:71:VAL:HG22	1:B:97:ILE:HB	1.89	0.54
1:F:86:SER:HB3	1:F:89:VAL:HG12	1.90	0.53
1:F:85:ASN:HB3	1:G:85:ASN:ND2	2.23	0.53
1:G:55:GLN:OE1	1:G:93:GLU:N	2.28	0.53
1:I:74:ASP:HB3	1:I:78:VAL:CG1	2.38	0.53
1:I:87:PRO:HG2	1:I:88:ALA:N	2.23	0.53
1:G:103:THR:O	1:G:107:GLN:HG3	2.08	0.53
1:G:156:GLN:O	1:G:159:ARG:HB3	2.08	0.53
1:H:9:PRO:HA	1:H:26:GLU:OE1	2.07	0.53
1:D:49:THR:HG22	1:D:53:ASP:OD2	2.08	0.53
1:F:85:ASN:HD22	1:G:85:ASN:ND2	2.06	0.53
1:H:161:ASN:N	1:H:162:PRO:HD3	2.24	0.53
1:H:87:PRO:HG2	1:H:88:ALA:H	1.74	0.53
1:C:35:ILE:O	1:C:35:ILE:HG12	2.07	0.53
1:D:87:PRO:HG2	1:D:88:ALA:H	1.74	0.53
1:G:51:LEU:HB3	1:G:92:ILE:HD11	1.90	0.53
1:J:145:ALA:O	1:J:148:LEU:HB2	2.08	0.53
1:D:165:VAL:O	1:D:166:CYS:HB2	2.06	0.53
1:B:85:ASN:ND2	1:C:85:ASN:ND2	2.52	0.53
1:C:86:SER:HB3	1:C:89:VAL:CG1	2.39	0.53
1:D:43:PHE:CE2	1:D:78:VAL:HG23	2.44	0.53
1:E:124:ILE:HB	1:E:133:ALA:HB3	1.91	0.53
1:F:15:PHE:CE1	1:F:80:LYS:HD2	2.44	0.53
1:J:101:SER:O	1:J:102:GLN:HB2	2.07	0.53
1:D:11:ARG:HD2	1:D:23:GLU:OE1	2.08	0.53
1:J:165:VAL:O	1:J:166:CYS:HB2	2.09	0.53
1:E:42:ASP:OD2	1:E:79:HIS:ND1	2.40	0.52
1:G:33:TRP:CE2	1:G:156:GLN:HG2	2.45	0.52
1:C:89:VAL:HG23	1:C:92:ILE:HD12	1.90	0.52
1:D:110:VAL:HG13	1:D:110:VAL:O	2.09	0.52
1:D:35:ILE:O	1:D:35:ILE:HG12	2.08	0.52
1:E:87:PRO:HG2	1:E:88:ALA:H	1.74	0.52
1:E:140:GLY:HA2	1:F:165:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:131:ILE:HD12	1:I:131:ILE:N	2.24	0.52
1:B:21:PHE:CD1	1:B:76:HIS:HD2	2.27	0.52
1:E:59:ALA:HA	1:E:62:LYS:HE2	1.92	0.52
1:E:46:VAL:HG21	1:E:120:ARG:NH2	2.25	0.52
1:F:156:GLN:O	1:F:159:ARG:HB3	2.09	0.52
1:H:50:GLU:O	1:H:54:VAL:HG23	2.09	0.52
1:J:33:TRP:CE2	1:J:127:PRO:HD3	2.45	0.52
1:B:46:VAL:HG21	1:B:120:ARG:HH22	1.74	0.52
1:A:138:ALA:HB2	1:B:3:ILE:HD11	1.92	0.52
1:G:7:VAL:HG21	1:G:125:ILE:HD13	1.91	0.52
1:H:16:GLN:OE1	1:H:19:LYS:HE3	2.09	0.52
1:H:26:GLU:H	1:H:26:GLU:CD	2.13	0.52
1:I:110:VAL:HG22	1:I:119:ASP:HB2	1.90	0.52
1:G:137:ASN:ND2	1:G:143:ARG:HG2	2.25	0.52
1:D:22:PHE:N	1:D:22:PHE:CD2	2.78	0.52
1:A:51:LEU:HB3	1:A:92:ILE:HD11	1.92	0.51
1:E:71:VAL:HG22	1:E:97:ILE:HB	1.92	0.51
1:H:33:TRP:CZ3	1:H:126:ASP:HA	2.46	0.51
1:D:33:TRP:CB	1:D:66:VAL:HG22	2.40	0.51
1:J:128:ASP:OD2	1:J:159:ARG:NH1	2.43	0.51
1:H:53:ASP:HA	1:H:56:LYS:HD2	1.91	0.51
1:J:67:GLU:OE1	1:J:67:GLU:HA	2.10	0.51
1:B:25:THR:C	1:B:27:ALA:N	2.63	0.51
1:A:165:VAL:HG21	1:B:140:GLY:HA2	1.93	0.51
1:H:57:GLU:C	1:H:61:LEU:HD12	2.31	0.51
1:I:89:VAL:HG23	1:I:92:ILE:HD12	1.92	0.51
1:F:54:VAL:HG12	1:F:94:TYR:CE2	2.46	0.51
1:G:112:ASN:HD21	1:G:114:GLU:CG	2.23	0.51
1:H:101:SER:O	1:H:102:GLN:HB2	2.11	0.51
1:H:33:TRP:CE3	1:H:126:ASP:HA	2.45	0.51
1:I:161:ASN:N	1:I:162:PRO:HD3	2.26	0.51
1:C:86:SER:HB3	1:C:89:VAL:HG12	1.94	0.51
1:E:148:LEU:O	1:E:152:VAL:HG13	2.11	0.51
1:F:154:ALA:O	1:F:158:VAL:HG23	2.11	0.51
1:A:85:ASN:HB3	1:J:85:ASN:ND2	2.26	0.50
1:A:87:PRO:HG2	1:A:88:ALA:H	1.76	0.50
1:D:154:ALA:O	1:D:158:VAL:HG23	2.11	0.50
1:E:60:GLU:HG2	1:E:63:LYS:NZ	2.25	0.50
1:F:99:ASP:CG	1:F:104:ILE:HG23	2.31	0.50
1:C:71:VAL:HG22	1:C:97:ILE:HB	1.94	0.50
1:G:69:TYR:CD1	1:G:97:ILE:HD11	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ARG:HG2	1:C:120:ARG:HH11	1.74	0.50
1:D:75:THR:O	1:D:78:VAL:HG13	2.12	0.50
1:I:66:VAL:HG21	1:I:152:VAL:HG21	1.93	0.50
1:E:69:TYR:CD1	1:E:95:ILE:HB	2.47	0.50
1:F:132:GLN:HA	1:F:132:GLN:NE2	2.26	0.50
1:D:145:ALA:O	1:D:148:LEU:HB2	2.11	0.50
1:D:86:SER:HB3	1:D:89:VAL:CG1	2.42	0.50
1:H:112:ASN:C	1:H:112:ASN:ND2	2.65	0.50
1:I:49:THR:HG22	1:I:53:ASP:OD2	2.11	0.50
1:B:2:LEU:C	1:B:5:THR:HG23	2.32	0.50
1:C:10:PHE:C	1:C:10:PHE:CD1	2.85	0.50
1:G:3:ILE:O	1:G:3:ILE:HG23	2.11	0.50
1:B:25:THR:OG1	1:B:27:ALA:HB3	2.11	0.50
1:A:25:THR:OG1	1:A:27:ALA:HB3	2.12	0.50
1:A:75:THR:O	1:A:78:VAL:HG12	2.11	0.49
1:E:33:TRP:CD2	1:E:127:PRO:HD3	2.47	0.49
1:G:120:ARG:NH1	1:G:120:ARG:HG2	2.27	0.49
1:B:35:ILE:HD11	1:B:148:LEU:HG	1.93	0.49
1:G:165:VAL:HG11	1:H:140:GLY:HA2	1.94	0.49
1:J:2:LEU:O	1:J:5:THR:HG23	2.12	0.49
1:J:67:GLU:HG3	1:J:69:TYR:CE2	2.47	0.49
1:E:60:GLU:HA	1:E:63:LYS:HE3	1.94	0.49
1:J:76:HIS:HA	1:J:79:HIS:HD2	1.76	0.49
1:D:33:TRP:CE2	1:D:127:PRO:HD3	2.47	0.49
1:D:43:PHE:HE2	1:D:78:VAL:HG23	1.77	0.49
1:I:101:SER:O	1:I:102:GLN:HB2	2.11	0.49
1:A:97:ILE:HG22	1:A:98:GLY:N	2.27	0.49
1:C:39:TYR:CZ	1:C:72:SER:HB3	2.48	0.49
1:E:38:PHE:CD1	1:E:71:VAL:HB	2.47	0.49
1:I:58:TYR:CZ	1:I:62:LYS:HE2	2.47	0.49
1:G:15:PHE:HB2	1:G:21:PHE:CE1	2.48	0.49
1:D:22:PHE:HZ	1:D:95:ILE:HD12	1.78	0.49
1:C:47:CYS:H	1:D:166:CYS:HB3	1.77	0.49
1:F:50:GLU:OE1	1:F:120:ARG:NH1	2.46	0.49
1:D:110:VAL:HG22	1:D:119:ASP:HB2	1.95	0.49
1:I:131:ILE:H	1:I:131:ILE:HD12	1.78	0.49
1:E:26:GLU:CD	1:E:26:GLU:H	2.16	0.49
1:B:152:VAL:O	1:B:156:GLN:HG3	2.13	0.48
1:E:80:LYS:O	1:E:84:GLU:HG3	2.13	0.48
1:I:165:VAL:O	1:I:166:CYS:HB2	2.13	0.48
1:I:140:GLY:HA2	1:J:165:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:112:ASN:HD21	1:J:114:GLU:CG	2.25	0.48
1:E:145:ALA:HA	1:E:148:LEU:HD13	1.95	0.48
1:A:147:THR:HA	1:A:150:ASN:HD22	1.78	0.48
1:E:9:PRO:HA	1:E:26:GLU:OE1	2.14	0.48
1:G:112:ASN:C	1:G:112:ASN:ND2	2.53	0.48
1:C:26:GLU:O	1:C:29:LEU:HB2	2.14	0.48
1:D:55:GLN:OE1	1:D:93:GLU:N	2.41	0.48
1:J:9:PRO:HA	1:J:26:GLU:OE1	2.13	0.48
1:A:101:SER:O	1:A:102:GLN:HB2	2.13	0.48
1:A:110:VAL:CG2	1:A:119:ASP:HB2	2.41	0.48
1:A:156:GLN:O	1:A:159:ARG:HB3	2.13	0.48
1:A:32:LYS:NZ	1:A:34:SER:HB3	2.29	0.48
1:B:146:SER:O	1:B:149:ILE:HG12	2.14	0.48
1:G:141:ILE:HD12	1:G:141:ILE:H	1.79	0.48
1:B:33:TRP:CE2	1:B:127:PRO:HD3	2.49	0.48
1:D:22:PHE:N	1:D:22:PHE:HD2	2.12	0.48
1:D:74:ASP:HB3	1:D:78:VAL:CG1	2.44	0.48
1:E:69:TYR:CE1	1:E:95:ILE:HG13	2.49	0.48
1:H:125:ILE:HD12	1:H:125:ILE:N	2.28	0.47
1:C:141:ILE:HD12	1:C:141:ILE:N	2.29	0.47
1:D:5:THR:O	1:D:131:ILE:HD12	2.14	0.47
1:G:102:GLN:HE21	1:G:106:ARG:NH2	2.12	0.47
1:A:25:THR:C	1:A:27:ALA:N	2.68	0.47
1:F:85:ASN:HD22	1:G:85:ASN:CB	2.27	0.47
1:J:35:ILE:O	1:J:35:ILE:HG12	2.13	0.47
1:J:49:THR:HG22	1:J:53:ASP:OD2	2.14	0.47
1:F:85:ASN:HD22	1:G:85:ASN:HB3	1.77	0.47
1:H:53:ASP:N	1:H:56:LYS:HZ2	2.13	0.47
1:H:71:VAL:HG11	1:H:104:ILE:HD11	1.96	0.47
1:J:71:VAL:HG22	1:J:97:ILE:HB	1.94	0.47
1:A:140:GLY:HA2	1:B:165:VAL:HG11	1.97	0.47
1:B:85:ASN:HB3	1:C:85:ASN:ND2	2.30	0.47
1:D:74:ASP:HB3	1:D:78:VAL:HG11	1.97	0.47
1:H:86:SER:HB3	1:H:89:VAL:CG1	2.44	0.47
1:J:87:PRO:HG2	1:J:88:ALA:N	2.26	0.47
1:C:145:ALA:O	1:C:148:LEU:HB2	2.14	0.47
1:D:120:ARG:HG2	1:D:120:ARG:NH1	2.29	0.47
1:D:52:GLU:O	1:D:56:LYS:HG3	2.14	0.47
1:E:11:ARG:HD2	1:E:23:GLU:OE1	2.14	0.47
1:F:33:TRP:CE2	1:F:127:PRO:HD3	2.50	0.47
1:C:51:LEU:HD12	1:C:94:TYR:OH	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:ARG:HD2	1:F:23:GLU:CD	2.35	0.47
1:G:7:VAL:HG11	1:G:29:LEU:HD12	1.96	0.47
1:G:33:TRP:CE2	1:G:127:PRO:HD3	2.50	0.47
1:G:86:SER:HB3	1:G:89:VAL:HG12	1.97	0.47
1:B:38:PHE:CD1	1:B:71:VAL:HB	2.50	0.46
1:B:33:TRP:HB3	1:B:66:VAL:HG22	1.96	0.46
1:I:10:PHE:CE2	1:I:26:GLU:HA	2.51	0.46
1:J:101:SER:OG	1:J:103:THR:HG23	2.16	0.46
1:F:110:VAL:HG13	1:F:110:VAL:O	2.15	0.46
1:H:2:LEU:HB3	1:H:131:ILE:HD12	1.98	0.46
1:A:32:LYS:HZ1	1:A:34:SER:HB3	1.79	0.46
1:E:33:TRP:CE2	1:E:127:PRO:HD3	2.51	0.46
1:F:7:VAL:CG2	1:F:125:ILE:HD13	2.44	0.46
1:G:58:TYR:CE1	1:G:62:LYS:HE2	2.50	0.46
1:C:53:ASP:HA	1:C:56:LYS:HD2	1.97	0.46
1:D:33:TRP:HB3	1:D:66:VAL:HG22	1.98	0.46
1:G:67:GLU:OE1	1:G:67:GLU:HA	2.15	0.46
1:B:51:LEU:O	1:B:94:TYR:OH	2.32	0.46
1:F:35:ILE:HG23	1:F:68:VAL:HG22	1.97	0.46
1:H:33:TRP:CD2	1:H:127:PRO:HD3	2.51	0.46
1:J:69:TYR:N	1:J:69:TYR:CD2	2.84	0.46
1:H:3:ILE:HD11	1:H:132:GLN:C	2.36	0.46
1:H:92:ILE:HG23	1:H:94:TYR:CZ	2.50	0.46
1:B:22:PHE:HZ	1:B:95:ILE:HD12	1.80	0.46
1:H:35:ILE:HG22	1:H:66:VAL:CG1	2.45	0.46
1:H:80:LYS:O	1:H:84:GLU:HG3	2.16	0.46
1:H:53:ASP:HA	1:H:56:LYS:NZ	2.31	0.46
1:I:19:LYS:H	1:I:19:LYS:HD2	1.81	0.46
1:G:116:GLY:C	1:G:117:LEU:HD23	2.36	0.46
1:I:138:ALA:HB2	1:J:3:ILE:HD11	1.98	0.46
1:G:102:GLN:NE2	1:G:106:ARG:NH2	2.64	0.45
1:A:146:SER:O	1:A:149:ILE:HG12	2.16	0.45
1:D:44:SER:OG	1:D:46:VAL:HG22	2.17	0.45
1:F:26:GLU:N	1:F:26:GLU:OE1	2.40	0.45
1:H:53:ASP:CA	1:H:56:LYS:HD2	2.46	0.45
1:I:154:ALA:O	1:I:158:VAL:HG23	2.16	0.45
1:B:148:LEU:O	1:B:152:VAL:HG13	2.16	0.45
1:E:15:PHE:CD1	1:E:16:GLN:N	2.84	0.45
1:G:152:VAL:O	1:G:156:GLN:HG3	2.17	0.45
1:H:16:GLN:CD	1:H:95:ILE:HD13	2.37	0.45
1:I:47:CYS:C	1:I:49:THR:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:64:LEU:HD22	1:J:156:GLN:HE22	1.81	0.45
1:A:43:PHE:CZ	1:A:82:TRP:HA	2.51	0.45
1:E:16:GLN:CD	1:E:95:ILE:HD13	2.37	0.45
1:J:43:PHE:CZ	1:J:82:TRP:HA	2.51	0.45
1:A:122:THR:OG1	1:A:143:ARG:HD2	2.16	0.45
1:A:3:ILE:HG23	1:A:3:ILE:O	2.16	0.45
1:B:101:SER:O	1:B:102:GLN:HB2	2.17	0.45
1:D:47:CYS:C	1:D:49:THR:H	2.19	0.45
1:H:89:VAL:HG23	1:H:92:ILE:HD12	1.97	0.45
1:A:89:VAL:HG23	1:A:92:ILE:HD12	1.98	0.45
1:C:55:GLN:NE2	1:C:93:GLU:HG3	2.32	0.45
1:A:25:THR:C	1:A:27:ALA:H	2.20	0.45
1:B:36:VAL:HG12	1:B:125:ILE:HD11	1.98	0.45
1:E:101:SER:O	1:E:102:GLN:HB2	2.16	0.45
1:F:39:TYR:OH	1:F:79:HIS:CE1	2.70	0.44
1:B:35:ILE:HG23	1:B:68:VAL:HG22	2.00	0.44
1:D:152:VAL:O	1:D:156:GLN:HG3	2.17	0.44
1:E:165:VAL:O	1:E:165:VAL:HG12	2.17	0.44
1:F:47:CYS:C	1:F:49:THR:H	2.20	0.44
1:B:87:PRO:HG2	1:B:88:ALA:N	2.32	0.44
1:H:110:VAL:HG22	1:H:119:ASP:HB2	1.99	0.44
1:D:101:SER:O	1:D:102:GLN:HB2	2.18	0.44
1:A:140:GLY:HA2	1:B:165:VAL:HG21	2.00	0.44
1:A:39:TYR:CZ	1:A:72:SER:HB3	2.53	0.44
1:C:112:ASN:OD1	1:C:115:THR:HG23	2.17	0.44
1:F:138:ALA:HB3	1:F:141:ILE:HD13	1.99	0.44
1:F:165:VAL:O	1:F:166:CYS:CB	2.63	0.44
1:F:21:PHE:CD1	1:F:76:HIS:HD2	2.35	0.44
1:G:2:LEU:C	1:G:5:THR:HG23	2.38	0.44
1:I:11:ARG:HD2	1:I:23:GLU:CD	2.38	0.44
1:I:21:PHE:CD1	1:I:76:HIS:HD2	2.36	0.44
1:G:15:PHE:HB2	1:G:21:PHE:HE1	1.81	0.44
1:H:53:ASP:N	1:H:56:LYS:NZ	2.66	0.44
1:E:33:TRP:CE3	1:E:126:ASP:HA	2.52	0.44
1:H:50:GLU:OE1	1:H:120:ARG:NH1	2.51	0.44
1:H:51:LEU:HD22	1:H:51:LEU:H	1.83	0.44
1:A:37:VAL:HG23	1:A:37:VAL:O	2.16	0.44
1:B:41:ALA:O	1:B:44:SER:HB2	2.18	0.44
1:I:55:GLN:NE2	1:I:93:GLU:HG3	2.33	0.44
1:A:138:ALA:CB	1:B:132:GLN:NE2	2.81	0.43
1:J:112:ASN:ND2	1:J:114:GLU:HG3	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:VAL:HG11	1:B:29:LEU:HD12	1.99	0.43
1:E:35:ILE:O	1:E:35:ILE:HG23	2.18	0.43
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.83	0.43
1:B:20:ASP:OD1	1:B:21:PHE:N	2.51	0.43
1:C:47:CYS:C	1:C:49:THR:H	2.22	0.43
1:F:85:ASN:ND2	1:G:85:ASN:ND2	2.65	0.43
1:J:158:VAL:HG22	1:J:165:VAL:HG22	2.01	0.43
1:F:35:ILE:HG22	1:F:66:VAL:CG1	2.48	0.43
1:I:74:ASP:HB3	1:I:78:VAL:HG13	1.99	0.43
1:A:47:CYS:C	1:A:49:THR:H	2.21	0.43
1:J:11:ARG:HD2	1:J:23:GLU:CD	2.39	0.43
1:J:86:SER:CB	1:J:89:VAL:HG12	2.49	0.43
1:J:55:GLN:OE1	1:J:92:ILE:HA	2.19	0.43
1:H:47:CYS:C	1:H:49:THR:H	2.22	0.43
1:J:87:PRO:CG	1:J:88:ALA:H	2.31	0.43
1:D:131:ILE:HD12	1:D:131:ILE:H	1.83	0.43
1:J:26:GLU:HG2	1:J:27:ALA:H	1.82	0.43
1:C:149:ILE:O	1:C:153:LYS:HG3	2.18	0.43
1:E:102:GLN:NE2	1:E:106:ARG:HH22	2.17	0.43
1:G:147:THR:HA	1:G:150:ASN:HD22	1.84	0.43
1:I:87:PRO:CG	1:I:88:ALA:H	2.30	0.43
1:J:106:ARG:NH1	1:J:111:LEU:HD22	2.34	0.43
1:J:47:CYS:C	1:J:49:THR:H	2.22	0.43
1:D:33:TRP:HB2	1:D:66:VAL:HG22	2.01	0.43
1:G:101:SER:O	1:G:102:GLN:HB2	2.19	0.43
1:B:47:CYS:C	1:B:49:THR:H	2.22	0.42
1:D:120:ARG:HG2	1:D:120:ARG:HH11	1.84	0.42
1:E:39:TYR:HE2	1:E:42:ASP:OD1	2.02	0.42
1:I:71:VAL:HG21	1:I:104:ILE:HD11	2.01	0.42
1:C:144:ASP:OD1	1:C:146:SER:OG	2.29	0.42
1:C:3:ILE:O	1:C:3:ILE:HG23	2.17	0.42
1:E:149:ILE:HG13	1:E:150:ASN:N	2.33	0.42
1:E:13:GLN:HB2	1:E:76:HIS:ND1	2.34	0.42
1:H:165:VAL:HG12	1:H:165:VAL:O	2.19	0.42
1:A:9:PRO:HA	1:A:26:GLU:OE1	2.19	0.42
1:C:165:VAL:HG11	1:D:140:GLY:HA2	2.02	0.42
1:D:22:PHE:CZ	1:D:95:ILE:HD12	2.55	0.42
1:B:102:GLN:HE21	1:B:106:ARG:NH2	2.17	0.42
1:A:21:PHE:CD1	1:A:76:HIS:HD2	2.37	0.42
1:C:16:GLN:CD	1:C:95:ILE:HD13	2.40	0.42
1:C:75:THR:OG1	1:C:78:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:PHE:CZ	1:C:95:ILE:HD12	2.52	0.42
1:E:47:CYS:C	1:E:49:THR:H	2.23	0.42
1:G:7:VAL:CG2	1:G:125:ILE:HD13	2.50	0.42
1:J:112:ASN:HD22	1:J:115:THR:H	1.66	0.42
1:A:163:GLY:C	1:A:165:VAL:H	2.23	0.42
1:B:112:ASN:C	1:B:112:ASN:ND2	2.72	0.42
1:D:25:THR:C	1:D:27:ALA:N	2.71	0.42
1:F:145:ALA:O	1:F:148:LEU:HB2	2.19	0.42
1:I:49:THR:O	1:I:52:GLU:HG2	2.20	0.42
1:I:74:ASP:HB3	1:I:78:VAL:HG11	2.02	0.42
1:A:147:THR:HA	1:A:150:ASN:ND2	2.34	0.42
1:D:7:VAL:CG2	1:D:125:ILE:HD13	2.49	0.42
1:D:3:ILE:HG23	1:D:3:ILE:O	2.20	0.42
1:G:39:TYR:CE2	1:G:42:ASP:OD1	2.73	0.42
1:G:49:THR:HG22	1:G:53:ASP:OD2	2.20	0.42
1:D:20:ASP:O	1:D:21:PHE:C	2.58	0.42
1:I:86:SER:HB3	1:I:89:VAL:CG1	2.50	0.42
1:B:33:TRP:CE3	1:B:126:ASP:HA	2.55	0.41
1:B:20:ASP:O	1:B:21:PHE:C	2.59	0.41
1:C:19:LYS:H	1:C:19:LYS:CD	2.30	0.41
1:C:29:LEU:HD23	1:C:29:LEU:HA	1.86	0.41
1:F:161:ASN:N	1:F:162:PRO:CD	2.82	0.41
1:F:163:GLY:C	1:F:165:VAL:H	2.21	0.41
1:F:25:THR:OG1	1:F:27:ALA:HB3	2.19	0.41
1:F:43:PHE:CZ	1:F:82:TRP:HA	2.55	0.41
1:H:26:GLU:CD	1:H:26:GLU:N	2.72	0.41
1:I:87:PRO:CG	1:I:88:ALA:N	2.83	0.41
1:J:10:PHE:C	1:J:10:PHE:CD1	2.93	0.41
1:J:163:GLY:C	1:J:165:VAL:H	2.24	0.41
1:D:147:THR:O	1:D:151:LYS:HG3	2.20	0.41
1:C:140:GLY:CA	1:D:158:VAL:HG21	2.41	0.41
1:F:22:PHE:HZ	1:F:95:ILE:HD12	1.85	0.41
1:C:51:LEU:HB3	1:C:92:ILE:HD11	2.03	0.41
1:D:15:PHE:CE2	1:D:80:LYS:HA	2.55	0.41
1:G:161:ASN:N	1:G:162:PRO:CD	2.81	0.41
1:H:163:GLY:C	1:H:165:VAL:H	2.24	0.41
1:E:82:TRP:CE2	1:E:89:VAL:HG11	2.56	0.41
1:G:66:VAL:CG2	1:G:152:VAL:HG21	2.46	0.41
1:I:99:ASP:OD1	1:I:104:ILE:HG23	2.19	0.41
1:A:120:ARG:HG2	1:A:120:ARG:NH1	2.35	0.41
1:B:145:ALA:O	1:B:148:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:THR:O	1:D:78:VAL:CG1	2.68	0.41
1:G:138:ALA:CB	1:H:132:GLN:HE21	2.33	0.41
1:I:92:ILE:HG23	1:I:94:TYR:CE2	2.54	0.41
1:A:46:VAL:HG21	1:A:120:ARG:HH22	1.86	0.41
1:A:68:VAL:O	1:A:94:TYR:HB2	2.20	0.41
1:D:10:PHE:O	1:D:25:THR:HA	2.21	0.41
1:F:165:VAL:O	1:F:166:CYS:HB2	2.21	0.41
1:J:74:ASP:HB3	1:J:78:VAL:HG13	2.03	0.41
1:C:33:TRP:HB3	1:C:66:VAL:HG22	2.01	0.41
1:F:19:LYS:H	1:F:19:LYS:HD2	1.86	0.41
1:F:16:GLN:CD	1:F:95:ILE:HD13	2.41	0.41
1:B:3:ILE:HG23	1:B:3:ILE:O	2.21	0.41
1:D:75:THR:OG1	1:D:78:VAL:HG12	2.20	0.41
1:G:69:TYR:HD1	1:G:97:ILE:HD11	1.83	0.41
1:I:140:GLY:HA2	1:J:165:VAL:CG1	2.50	0.41
1:A:112:ASN:OD1	1:A:115:THR:HG23	2.21	0.41
1:B:86:SER:HB3	1:B:89:VAL:HG12	2.02	0.41
1:C:163:GLY:C	1:C:165:VAL:H	2.23	0.41
1:C:26:GLU:HG2	1:C:27:ALA:N	2.36	0.41
1:E:20:ASP:O	1:E:21:PHE:C	2.59	0.41
1:F:15:PHE:CD1	1:F:80:LYS:HD2	2.55	0.41
1:F:21:PHE:HE2	1:G:45:PHE:CZ	2.39	0.41
1:G:47:CYS:C	1:G:49:THR:H	2.24	0.41
1:H:102:GLN:HE21	1:H:106:ARG:HH22	1.68	0.41
1:J:51:LEU:HB3	1:J:92:ILE:HD11	2.03	0.41
1:A:87:PRO:HG2	1:A:88:ALA:N	2.35	0.41
1:I:166:CYS:HB3	1:J:47:CYS:H	1.86	0.41
1:A:19:LYS:HG3	1:A:19:LYS:H	1.56	0.41
1:E:22:PHE:CZ	1:E:95:ILE:HD12	2.53	0.41
1:H:52:GLU:O	1:H:55:GLN:HB3	2.21	0.41
1:I:20:ASP:O	1:I:21:PHE:C	2.59	0.41
1:I:33:TRP:CD2	1:I:127:PRO:HD3	2.56	0.41
1:A:33:TRP:CE3	1:A:126:ASP:HA	2.56	0.40
1:D:97:ILE:HG22	1:D:98:GLY:N	2.36	0.40
1:E:68:VAL:O	1:E:94:TYR:HB2	2.21	0.40
1:H:43:PHE:CE2	1:H:78:VAL:HG23	2.56	0.40
1:A:20:ASP:OD1	1:A:21:PHE:N	2.54	0.40
1:B:149:ILE:HG13	1:B:150:ASN:N	2.36	0.40
1:G:58:TYR:CE2	1:G:94:TYR:HB3	2.56	0.40
1:H:68:VAL:O	1:H:94:TYR:HB2	2.21	0.40
1:I:163:GLY:C	1:I:165:VAL:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3:ILE:O	1:I:3:ILE:CG2	2.69	0.40
1:A:165:VAL:HG12	1:A:165:VAL:O	2.22	0.40
1:B:126:ASP:OD1	1:B:126:ASP:C	2.59	0.40
1:C:20:ASP:O	1:C:21:PHE:C	2.60	0.40
1:F:60:GLU:OE2	1:F:63:LYS:HD2	2.22	0.40
1:H:20:ASP:O	1:H:21:PHE:C	2.59	0.40
1:I:33:TRP:HB3	1:I:66:VAL:HG22	2.03	0.40
1:I:35:ILE:HG22	1:I:66:VAL:HG13	2.03	0.40
1:J:102:GLN:HE21	1:J:102:GLN:HB2	1.63	0.40
1:C:49:THR:HG22	1:C:50:GLU:N	2.37	0.40
1:G:163:GLY:C	1:G:165:VAL:H	2.25	0.40
1:G:20:ASP:O	1:G:21:PHE:C	2.59	0.40
1:A:126:ASP:OD1	1:A:126:ASP:C	2.60	0.40
1:D:50:GLU:OE1	1:D:120:ARG:NH1	2.54	0.40
1:F:121:GLY:HA2	1:F:135:GLU:O	2.21	0.40
1:F:95:ILE:H	1:F:95:ILE:HG12	1.68	0.40
1:J:20:ASP:O	1:J:21:PHE:C	2.60	0.40
1:J:45:PHE:HD1	1:J:45:PHE:HA	1.78	0.40
1:J:8:GLN:HA	1:J:9:PRO:HD3	1.95	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	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	7	27
1	B	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	7	27
1	C	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	7	27
1	D	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	7	27
1	E	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	7	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	164/187 (88%)	145 (88%)	15 (9%)	4 (2%)	7	27
1	G	164/187 (88%)	145 (88%)	15 (9%)	4 (2%)	7	27
1	H	164/187 (88%)	144 (88%)	16 (10%)	4 (2%)	7	27
1	I	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	7	27
1	J	164/187 (88%)	143 (87%)	17 (10%)	4 (2%)	7	27
All	All	1640/1870 (88%)	1437 (88%)	163 (10%)	40 (2%)	7	27

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	B	21	PHE
1	C	21	PHE
1	D	21	PHE
1	E	21	PHE
1	F	21	PHE
1	G	21	PHE
1	H	21	PHE
1	I	21	PHE
1	J	21	PHE
1	A	40	PRO
1	B	40	PRO
1	C	40	PRO
1	D	40	PRO
1	E	40	PRO
1	F	40	PRO
1	G	40	PRO
1	H	40	PRO
1	I	40	PRO
1	J	40	PRO
1	A	48	PRO
1	B	48	PRO
1	F	48	PRO
1	G	48	PRO
1	B	165	VAL
1	H	48	PRO
1	A	165	VAL
1	E	48	PRO
1	E	165	VAL
1	F	165	VAL

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Mol	Chain	Res	Type
1	I	48	PRO
1	J	48	PRO
1	C	48	PRO
1	C	165	VAL
1	D	48	PRO
1	H	165	VAL
1	G	165	VAL
1	I	165	VAL
1	J	165	VAL
1	D	165	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	141/158 (89%)	135 (96%)	6 (4%)	33	68
1	B	141/158 (89%)	132 (94%)	9 (6%)	20	50
1	C	141/158 (89%)	127 (90%)	14 (10%)	9	28
1	D	141/158 (89%)	130 (92%)	11 (8%)	15	39
1	E	141/158 (89%)	134 (95%)	7 (5%)	28	62
1	F	141/158 (89%)	132 (94%)	9 (6%)	20	50
1	G	141/158 (89%)	128 (91%)	13 (9%)	11	32
1	H	141/158 (89%)	129 (92%)	12 (8%)	12	35
1	I	141/158 (89%)	134 (95%)	7 (5%)	28	62
1	J	141/158 (89%)	129 (92%)	12 (8%)	12	35
All	All	1410/1580 (89%)	1310 (93%)	100 (7%)	17	44

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	32	LYS
1	A	35	ILE

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Mol	Chain	Res	Type
1	A	36	VAL
1	A	104	ILE
1	A	152	VAL
1	B	26	GLU
1	B	32	LYS
1	B	37	VAL
1	B	78	VAL
1	B	104	ILE
1	B	110	VAL
1	B	112	ASN
1	B	136	ILE
1	B	148	LEU
1	C	19	LYS
1	C	20	ASP
1	C	35	ILE
1	C	37	VAL
1	C	51	LEU
1	C	72	SER
1	C	73	THR
1	C	78	VAL
1	C	103	THR
1	C	104	ILE
1	C	110	VAL
1	C	112	ASN
1	C	148	LEU
1	C	166	CYS
1	D	22	PHE
1	D	26	GLU
1	D	32	LYS
1	D	35	ILE
1	D	70	SER
1	D	78	VAL
1	D	89	VAL
1	D	110	VAL
1	D	112	ASN
1	D	148	LEU
1	D	166	CYS
1	E	19	LYS
1	E	26	GLU
1	E	37	VAL
1	E	89	VAL
1	E	103	THR

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Mol	Chain	Res	Type
1	E	104	ILE
1	E	166	CYS
1	F	5	THR
1	F	19	LYS
1	F	28	ASP
1	F	35	ILE
1	F	78	VAL
1	F	104	ILE
1	F	110	VAL
1	F	112	ASN
1	F	166	CYS
1	G	19	LYS
1	G	20	ASP
1	G	35	ILE
1	G	36	VAL
1	G	51	LEU
1	G	72	SER
1	G	78	VAL
1	G	104	ILE
1	G	110	VAL
1	G	112	ASN
1	G	148	LEU
1	G	149	ILE
1	G	166	CYS
1	H	11	ARG
1	H	19	LYS
1	H	26	GLU
1	H	32	LYS
1	H	35	ILE
1	H	37	VAL
1	H	78	VAL
1	H	104	ILE
1	H	110	VAL
1	H	112	ASN
1	H	115	THR
1	H	166	CYS
1	I	19	LYS
1	I	20	ASP
1	I	35	ILE
1	I	36	VAL
1	I	104	ILE
1	I	152	VAL

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Mol	Chain	Res	Type
1	I	166	CYS
1	J	19	LYS
1	J	35	ILE
1	J	36	VAL
1	J	37	VAL
1	J	51	LEU
1	J	69	TYR
1	J	103	THR
1	J	104	ILE
1	J	110	VAL
1	J	112	ASN
1	J	148	LEU
1	J	166	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	85	ASN
1	A	102	GLN
1	A	150	ASN
1	A	156	GLN
1	B	85	ASN
1	B	102	GLN
1	B	132	GLN
1	B	156	GLN
1	C	112	ASN
1	C	156	GLN
1	D	102	GLN
1	D	112	ASN
1	D	132	GLN
1	D	156	GLN
1	E	83	HIS
1	E	85	ASN
1	E	102	GLN
1	E	150	ASN
1	E	156	GLN
1	F	79	HIS
1	F	85	ASN
1	F	102	GLN
1	F	112	ASN
1	F	132	GLN

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Mol	Chain	Res	Type
1	F	150	ASN
1	F	156	GLN
1	G	79	HIS
1	G	85	ASN
1	G	102	GLN
1	G	112	ASN
1	G	132	GLN
1	G	137	ASN
1	G	150	ASN
1	G	156	GLN
1	H	102	GLN
1	H	112	ASN
1	H	132	GLN
1	H	156	GLN
1	I	85	ASN
1	I	102	GLN
1	I	137	ASN
1	I	156	GLN
1	J	79	HIS
1	J	83	HIS
1	J	102	GLN
1	J	112	ASN
1	J	132	GLN
1	J	150	ASN
1	J	156	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

Of 2 ligands modelled in this entry, 2 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.