



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:47 AM UTC

PDB ID : 5WXV / pdb_00005wxv
Title : The crystal structure of VabB-ICL domain from *Vibrio anguillarum* 775
Authors : Du, J.; Ma, Q.
Deposited on : 2017-01-09
Resolution : 2.30 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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

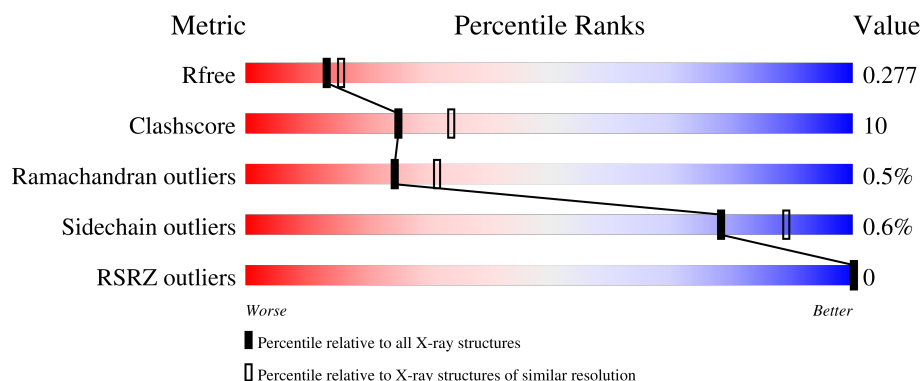
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	217	
1	B	217	
1	C	217	
1	D	217	
1	E	217	

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Mol	Chain	Length	Quality of chain
1	F	217	 71%20%9%
1	G	217	 72%18%9%
1	H	217	 74%17%9%
1	I	217	 78%13%9%
1	J	217	 68%23%9%
1	K	217	 70%21%9%
1	L	217	 67%24%9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19230 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 Isochorismate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	B	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	C	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	D	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	E	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	F	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	G	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	H	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	I	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	J	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	K	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			
1	L	198	Total	C	N	O	S	0	0	0
			1574	1015	263	292	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		
2	B	38	Total	O	0	0
			38	38		

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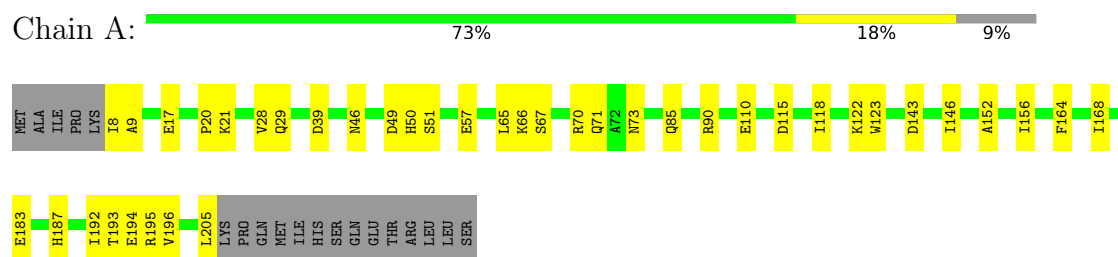
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	30	Total 30	O 30	0	0
2	D	37	Total 37	O 37	0	0
2	E	29	Total 29	O 29	0	0
2	F	25	Total 25	O 25	0	0
2	G	36	Total 36	O 36	0	0
2	H	31	Total 31	O 31	0	0
2	I	27	Total 27	O 27	0	0
2	J	20	Total 20	O 20	0	0
2	K	20	Total 20	O 20	0	0
2	L	15	Total 15	O 15	0	0

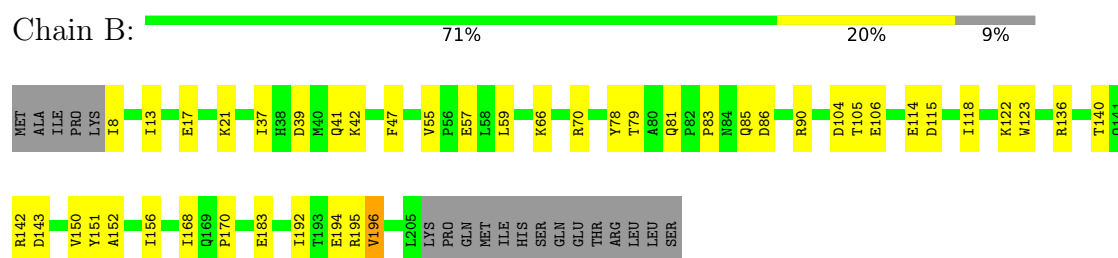
3 Residue-property plots

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.

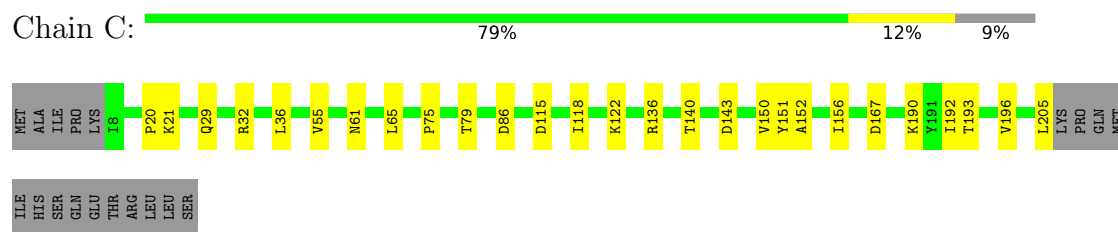
• Molecule 1: Isochorismate lyase



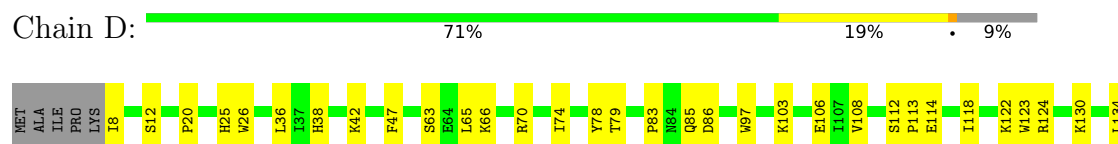
• Molecule 1: Isochorismate lyase



• Molecule 1: Isochorismate lyase



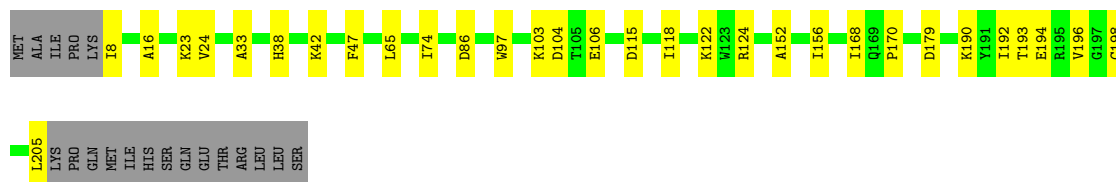
• Molecule 1: Isochorismate lyase





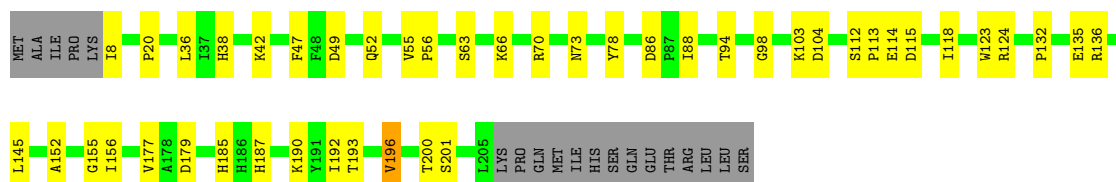
- Molecule 1: Isochorismate lyase

Chain E: 77% 14% 9%



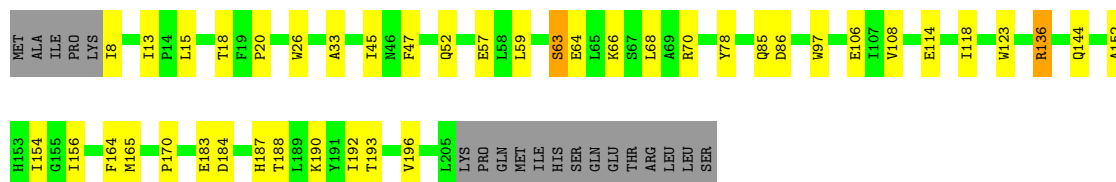
- Molecule 1: Isochorismate lyase

Chain F: 71% 20% 9%



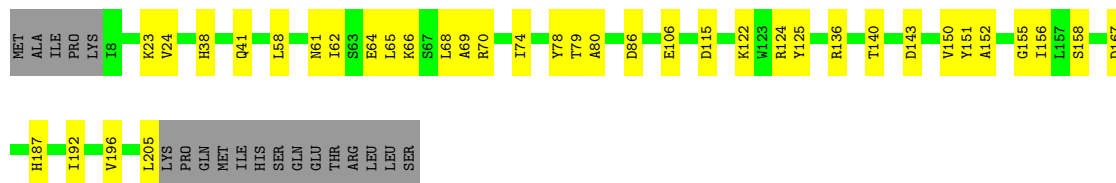
- Molecule 1: Isochorismate lyase

Chain G: 72% 18% 9%



- Molecule 1: Isochorismate lyase

Chain H: 74% 17% 9%



- Molecule 1: Isochorismate lyase

Chain I: 78% 13% 9%



PRO
GLN
MET
ILE
HIS
SER
GLN
GLU
THR
ARG
LEU
SER

• Molecule 1: Isochorismate lyase

Chain J:  68% 23% 9%

MET
ALA
ILE
PRO
LYS
I8
A9
S10
I13
P20
K23
L36
I37
H38
K42
A53
P54
P55
P56
E57
K66
R70
Q71
T79
N84
Q85
R90
T94
G98
D104
I107
E110
D115
G116
D117
I118
Q119
K122
H123
R124
K130

R136
E139
Q144
L145
V150
Y151
A152
G155
I156
I168
Q169
P170
F171
H185
T188
L189
K190
Y191
I192
T193
V196
L205
LYS
PRO
GLN
MET
ILE
HIS
SER
GLN
THR
ARG
LEU
SER

• Molecule 1: Isochorismate lyase

Chain K:  70% 21% 9%

MET
ALA
ILE
LYS
I8
P20
L36
K42
F47
H50
V55
P56
L65
K66
R70
N73
T79
P83
D86
P87
I88
E89
R90
W97
K103
D104
T105
V108
S109
D115
G116
D117
I118
K122
W123
R124
Y125
S126
P132
E135

R136
M137
L145
A152
I156
D162
I168
V172
K190
Y191
I192
T193
E194
R195
V196
L205
LYS
PRO
GLN
MET
ILE
HIS
SER
GLN
THR
ARG
LEU
SER

• Molecule 1: Isochorismate lyase

Chain L:  67% 24% 9%

MET
ALA
PRO
LYS
I8
A9
S10
L15
F19
P20
V24
H25
W26
H27
V28
L36
I37
H38
D39
M40
Q41
K42
A53
P54
V55
E57
I62
S63
E64
L68
A69
R70
N73
T79
P82
Q85
E89
R90
T94
L101
D104

I107
E110
D115
W123
R136
L145
I146
V150
Y151
A152
G155
I156
A163
D167
I168
Q169
P170
A178
E183
D184
H185
T188
L189
K190
Y191
I192
T193
V196
L205
LYS
PRO
GLN
MET
ILE
HIS
SER
GLN
THR
ARG
LEU
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.53Å 173.88Å 143.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 2.30 47.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.92-2.30) 99.5 (47.92-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.206 , 0.273 0.209 , 0.277	Depositor DCC
R_{free} test set	8022 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19230	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.40	0/1614	0.61	0/2199
1	B	0.42	0/1614	0.61	0/2199
1	C	0.39	1/1614 (0.1%)	0.57	0/2199
1	D	0.41	0/1614	0.63	0/2199
1	E	0.40	0/1614	0.60	0/2199
1	F	0.36	0/1614	0.58	0/2199
1	G	0.40	0/1614	0.62	0/2199
1	H	0.38	0/1614	0.59	0/2199
1	I	0.38	0/1614	0.56	0/2199
1	J	0.34	0/1614	0.58	0/2199
1	K	0.35	0/1614	0.57	0/2199
1	L	0.33	0/1614	0.57	0/2199
All	All	0.38	1/19368 (0.0%)	0.59	0/26388

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	55	VAL	CA-CB	5.16	1.57	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1574	0	1547	35	1
1	B	1574	0	1547	36	0
1	C	1574	0	1549	22	0
1	D	1574	0	1549	34	1
1	E	1574	0	1549	24	0
1	F	1574	0	1549	27	0
1	G	1574	0	1549	41	0
1	H	1574	0	1549	29	1
1	I	1574	0	1548	29	0
1	J	1574	0	1547	33	1
1	K	1574	0	1549	42	0
1	L	1574	0	1548	43	0
2	A	34	0	0	5	1
2	B	38	0	0	3	0
2	C	30	0	0	5	0
2	D	37	0	0	6	0
2	E	29	0	0	5	0
2	F	25	0	0	2	0
2	G	36	0	0	3	0
2	H	31	0	0	5	1
2	I	27	0	0	5	1
2	J	20	0	0	2	1
2	K	20	0	0	4	0
2	L	15	0	0	2	0
All	All	19230	0	18580	362	4

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 10.

All (362) 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:K:136:ARG:HH11	1:L:136:ARG:CZ	1.65	1.09
1:D:8:ILE:N	2:D:301:HOH:O	1.90	1.03
1:B:8:ILE:N	2:B:301:HOH:O	2.01	0.92
1:E:97:TRP:O	2:E:301:HOH:O	1.91	0.88
1:G:183:GLU:OE1	2:G:301:HOH:O	1.91	0.87
1:K:194:GLU:HG3	1:K:195:ARG:HG2	1.58	0.86
1:A:8:ILE:N	2:A:302:HOH:O	2.09	0.85
1:K:136:ARG:NH1	1:L:136:ARG:CZ	2.41	0.83
1:F:8:ILE:N	2:F:301:HOH:O	2.10	0.83
1:K:135:GLU:OE2	2:K:301:HOH:O	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LYS:NZ	1:B:78:TYR:OH	2.10	0.83
1:K:136:ARG:HD3	1:L:136:ARG:HH22	1.44	0.83
1:E:8:ILE:N	2:E:302:HOH:O	2.13	0.81
1:I:97:TRP:O	2:I:301:HOH:O	1.98	0.81
1:L:192:ILE:HA	1:L:196:VAL:HG13	1.62	0.81
1:I:41:GLN:HE22	1:I:81:GLN:H	1.26	0.81
1:G:165:MET:HE1	1:H:158:SER:OG	1.81	0.80
1:C:21:LYS:NZ	2:C:304:HOH:O	2.13	0.80
1:I:41:GLN:NE2	1:I:81:GLN:H	1.79	0.80
1:J:205:LEU:O	2:J:301:HOH:O	1.99	0.80
1:E:198:CYS:SG	2:E:326:HOH:O	2.39	0.80
1:J:192:ILE:HA	1:J:196:VAL:HG13	1.65	0.77
1:K:97:TRP:O	2:K:302:HOH:O	2.03	0.77
1:G:66:LYS:NZ	1:G:78:TYR:OH	2.14	0.77
1:K:136:ARG:HD3	1:L:136:ARG:NH2	1.99	0.77
1:K:8:ILE:N	2:K:303:HOH:O	2.18	0.76
1:D:74:ILE:O	2:D:302:HOH:O	2.04	0.76
1:K:118:ILE:HD13	1:K:136:ARG:HH21	1.51	0.75
1:D:97:TRP:O	2:D:303:HOH:O	2.05	0.74
1:G:136:ARG:HD3	1:I:88:ILE:HD13	1.70	0.73
1:K:136:ARG:HH11	1:L:136:ARG:NH2	1.87	0.73
1:A:29:GLN:NE2	2:A:305:HOH:O	2.23	0.72
1:L:24:VAL:HG11	1:L:26:TRP:CE2	2.25	0.72
1:A:205:LEU:O	2:A:301:HOH:O	2.08	0.71
1:B:90:ARG:O	2:B:302:HOH:O	2.07	0.71
1:B:192:ILE:HA	1:B:196:VAL:HG13	1.73	0.71
1:I:96:PHE:HA	1:J:23:LYS:CE	2.21	0.71
1:H:143:ASP:OD2	2:H:301:HOH:O	2.09	0.71
1:K:136:ARG:NH1	1:L:136:ARG:NH2	2.40	0.70
1:B:57:GLU:OE2	2:B:303:HOH:O	2.10	0.70
1:C:143:ASP:OD2	2:C:301:HOH:O	2.10	0.70
1:G:192:ILE:HD13	1:G:196:VAL:HG11	1.74	0.70
1:B:66:LYS:HE2	1:B:70:ARG:HH21	1.57	0.69
1:K:36:LEU:HD12	1:K:145:LEU:HD21	1.73	0.69
1:H:205:LEU:O	2:H:302:HOH:O	2.10	0.69
1:G:13:ILE:HD12	1:G:57:GLU:HG3	1.74	0.69
1:K:190:LYS:O	1:K:193:THR:HG22	1.92	0.69
1:C:167:ASP:OD1	2:C:303:HOH:O	2.11	0.69
1:L:42:LYS:HB3	1:L:104:ASP:HB3	1.75	0.69
1:F:70:ARG:HH22	1:F:114:GLU:HB2	1.57	0.68
1:G:86:ASP:HA	1:I:118:ILE:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LYS:HE2	1:D:70:ARG:NH2	2.09	0.67
1:H:167:ASP:OD1	2:H:303:HOH:O	2.11	0.67
1:L:110:GLU:OE2	1:L:110:GLU:N	2.25	0.67
1:D:20:PRO:HB2	1:D:193:THR:HG21	1.77	0.66
1:G:20:PRO:HB2	1:G:193:THR:HG21	1.76	0.66
1:E:16:ALA:O	2:E:303:HOH:O	2.14	0.66
1:G:136:ARG:HD3	1:I:88:ILE:CD1	2.26	0.66
1:C:32:ARG:NH1	2:C:302:HOH:O	2.28	0.66
1:L:167:ASP:OD1	2:L:301:HOH:O	2.14	0.65
1:D:86:ASP:HA	1:E:118:ILE:HD12	1.76	0.65
1:G:118:ILE:HD12	1:I:86:ASP:HA	1.78	0.65
1:I:175:ASP:OD2	2:I:302:HOH:O	2.13	0.65
1:L:85:GLN:OE1	1:L:90:ARG:NH1	2.28	0.65
1:F:66:LYS:HE3	1:F:78:TYR:OH	1.97	0.64
1:B:86:ASP:HA	1:C:118:ILE:HD12	1.79	0.64
1:H:66:LYS:NZ	1:H:78:TYR:OH	2.20	0.64
1:B:136:ARG:O	1:B:140:THR:HG22	1.98	0.64
1:A:17:GLU:HB2	1:B:21:LYS:HE3	1.80	0.63
1:C:29:GLN:NE2	2:C:302:HOH:O	2.11	0.63
1:J:115:ASP:CG	1:J:116:GLY:H	2.06	0.63
1:I:192:ILE:HD13	1:I:196:VAL:HG11	1.79	0.63
1:I:96:PHE:HA	1:J:23:LYS:HE3	1.81	0.62
1:K:132:PRO:HA	1:K:135:GLU:OE1	2.00	0.62
1:J:110:GLU:N	1:J:110:GLU:OE1	2.31	0.62
1:B:66:LYS:HE2	1:B:70:ARG:NH2	2.14	0.62
1:I:192:ILE:HA	1:I:196:VAL:CG1	2.30	0.62
1:D:25:HIS:CG	2:D:306:HOH:O	2.52	0.61
1:B:42:LYS:HG3	1:B:104:ASP:HB3	1.83	0.61
1:A:20:PRO:HB2	1:A:193:THR:HG21	1.82	0.61
1:B:37:ILE:HD11	1:B:66:LYS:HG3	1.83	0.61
1:F:73:ASN:ND2	2:F:303:HOH:O	2.33	0.60
1:A:194:GLU:HG3	1:A:195:ARG:NH1	2.16	0.60
1:G:192:ILE:HA	1:G:196:VAL:CG1	2.31	0.60
1:D:83:PRO:O	2:D:304:HOH:O	2.15	0.60
1:G:192:ILE:HA	1:G:196:VAL:HG12	1.83	0.60
1:J:85:GLN:OE1	1:J:90:ARG:NH1	2.32	0.60
1:G:59:LEU:O	1:G:63:SER:OG	2.19	0.60
1:A:46:ASN:HB2	2:A:311:HOH:O	2.01	0.59
1:G:57:GLU:HG2	2:G:311:HOH:O	2.01	0.59
1:A:143:ASP:HA	1:A:168:ILE:HD12	1.83	0.59
1:D:66:LYS:NZ	1:D:78:TYR:OH	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ILE:HD12	1:E:86:ASP:HA	1.84	0.59
1:L:57:GLU:CD	1:L:57:GLU:H	2.11	0.59
1:G:165:MET:HE2	1:H:125:TYR:HB2	1.84	0.58
1:E:190:LYS:O	1:E:193:THR:HG22	2.04	0.58
1:G:70:ARG:NH2	1:G:114:GLU:HB2	2.18	0.58
1:E:192:ILE:HD13	1:E:196:VAL:HG11	1.85	0.58
1:L:40:MET:HE2	1:L:62:ILE:HD12	1.86	0.58
1:B:118:ILE:HD12	1:C:86:ASP:HA	1.85	0.58
1:C:192:ILE:HA	1:C:196:VAL:CG1	2.33	0.58
1:G:8:ILE:HA	1:G:47:PHE:O	2.02	0.57
1:L:190:LYS:O	1:L:193:THR:HG22	2.03	0.57
1:D:134:LEU:HD22	1:D:166:LEU:HD13	1.85	0.57
1:J:190:LYS:O	1:J:193:THR:HG22	2.04	0.57
1:A:66:LYS:HE3	1:A:70:ARG:HH21	1.69	0.57
1:D:70:ARG:NH2	1:D:114:GLU:HB2	2.20	0.57
1:J:136:ARG:NH1	1:J:139:GLU:OE1	2.38	0.56
1:J:42:LYS:HB3	1:J:104:ASP:HB3	1.88	0.56
1:A:192:ILE:HA	1:A:196:VAL:CG1	2.36	0.56
1:E:23:LYS:HD2	1:E:194:GLU:HA	1.86	0.56
1:I:152:ALA:HB3	1:I:179:ASP:OD2	2.05	0.56
1:G:66:LYS:HE2	1:G:70:ARG:NH2	2.20	0.56
1:D:192:ILE:HA	1:D:196:VAL:HG13	1.86	0.56
1:E:192:ILE:HA	1:E:196:VAL:CG1	2.36	0.56
1:F:103:LYS:HG3	1:F:104:ASP:CG	2.31	0.56
1:E:152:ALA:HB3	1:E:179:ASP:OD2	2.06	0.56
1:C:65:LEU:HD11	1:C:205:LEU:HD23	1.86	0.56
1:K:152:ALA:HA	1:K:156:ILE:HB	1.86	0.56
1:H:192:ILE:HA	1:H:196:VAL:CG1	2.35	0.56
1:L:152:ALA:HA	1:L:156:ILE:HB	1.89	0.55
1:A:192:ILE:HD13	1:A:196:VAL:HG11	1.88	0.55
1:G:184:ASP:O	1:G:187:HIS:HD2	1.90	0.55
1:I:136:ARG:HG2	2:I:327:HOH:O	2.06	0.55
1:E:192:ILE:HA	1:E:196:VAL:HG12	1.89	0.55
1:A:21:LYS:HE3	1:B:17:GLU:HB2	1.89	0.54
1:D:8:ILE:HA	1:D:47:PHE:O	2.08	0.54
1:C:20:PRO:HB2	1:C:193:THR:HG21	1.89	0.54
1:I:64:GLU:O	1:I:68:LEU:HD12	2.07	0.54
1:A:194:GLU:HG3	1:A:195:ARG:CZ	2.37	0.54
1:D:123:TRP:HB3	1:D:130:LYS:HE3	1.89	0.54
1:G:136:ARG:CD	1:I:88:ILE:HD13	2.36	0.54
1:I:117:ASP:OD1	2:I:303:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:152:ALA:HB1	1:J:188:THR:HG21	1.90	0.54
1:F:132:PRO:HA	1:F:135:GLU:OE2	2.08	0.54
1:A:57:GLU:H	1:A:57:GLU:CD	2.11	0.54
1:I:192:ILE:HA	1:I:196:VAL:HG12	1.90	0.53
1:B:194:GLU:HG3	1:B:195:ARG:NH1	2.23	0.53
1:F:49:ASP:HB3	1:F:52:GLN:HB2	1.90	0.53
1:G:165:MET:CE	1:H:125:TYR:HB2	2.39	0.53
1:I:168:ILE:O	1:I:170:PRO:HD3	2.09	0.53
1:J:57:GLU:CD	1:J:57:GLU:H	2.16	0.53
1:C:190:LYS:O	1:C:193:THR:HG22	2.08	0.53
1:D:26:TRP:HZ3	1:D:170:PRO:HD2	1.74	0.52
1:G:26:TRP:HZ3	1:G:170:PRO:HD2	1.73	0.52
1:I:190:LYS:O	1:I:193:THR:HG22	2.09	0.52
1:A:192:ILE:HD13	1:A:196:VAL:CG1	2.39	0.52
1:J:66:LYS:HE3	1:J:70:ARG:CZ	2.39	0.52
1:F:152:ALA:HA	1:F:156:ILE:HB	1.91	0.52
1:A:85:GLN:HG2	1:A:123:TRP:CH2	2.45	0.51
1:F:192:ILE:HA	1:F:196:VAL:HG13	1.91	0.51
1:L:8:ILE:N	2:L:303:HOH:O	2.43	0.51
1:J:8:ILE:N	2:J:308:HOH:O	2.43	0.51
1:H:152:ALA:HA	1:H:156:ILE:HB	1.91	0.51
1:E:103:LYS:HE3	1:E:104:ASP:OD2	2.10	0.51
1:H:136:ARG:HE	1:H:140:THR:HG21	1.76	0.51
1:C:192:ILE:HA	1:C:196:VAL:HG12	1.92	0.50
1:E:152:ALA:HA	1:E:156:ILE:HB	1.92	0.50
1:K:83:PRO:HB3	1:K:105:THR:HG21	1.94	0.50
1:K:136:ARG:HD3	1:L:136:ARG:CZ	2.41	0.50
1:L:10:SER:OG	1:L:53:ALA:O	2.25	0.50
1:J:152:ALA:HA	1:J:156:ILE:HB	1.93	0.50
1:G:97:TRP:O	2:G:302:HOH:O	2.19	0.50
1:K:42:LYS:HB3	1:K:104:ASP:HB3	1.92	0.50
1:L:168:ILE:O	1:L:170:PRO:HD3	2.11	0.50
1:G:152:ALA:HA	1:G:156:ILE:HB	1.92	0.50
1:C:152:ALA:HA	1:C:156:ILE:HB	1.93	0.50
1:K:137:MET:HE2	1:K:168:ILE:HD12	1.93	0.50
1:F:190:LYS:O	1:F:193:THR:HG22	2.11	0.50
1:C:79:THR:HB	1:C:122:LYS:HD3	1.94	0.49
1:I:190:LYS:HE3	1:I:194:GLU:OE2	2.11	0.49
1:K:194:GLU:CG	1:K:195:ARG:HG2	2.38	0.49
1:B:41:GLN:CD	1:B:81:GLN:H	2.20	0.49
1:J:10:SER:OG	1:J:53:ALA:O	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:HIS:CD2	1:G:188:THR:N	2.80	0.49
1:L:152:ALA:HB1	1:L:188:THR:HG21	1.93	0.49
1:G:184:ASP:O	1:G:187:HIS:CD2	2.66	0.49
1:B:85:GLN:HG2	1:B:123:TRP:CH2	2.48	0.49
1:E:24:VAL:HG23	2:E:326:HOH:O	2.12	0.49
1:F:55:VAL:HB	1:F:56:PRO:HD3	1.95	0.49
1:H:79:THR:HB	1:H:122:LYS:HD3	1.94	0.49
1:B:13:ILE:HD12	1:B:57:GLU:HB2	1.94	0.48
1:E:8:ILE:HA	1:E:47:PHE:O	2.12	0.48
1:H:61:ASN:O	1:H:65:LEU:HB2	2.13	0.48
1:K:70:ARG:HG3	1:K:70:ARG:HH11	1.77	0.48
1:K:136:ARG:HD3	1:L:136:ARG:NH1	2.28	0.48
1:B:143:ASP:HA	1:B:168:ILE:HD12	1.96	0.48
1:B:152:ALA:HA	1:B:156:ILE:HB	1.96	0.48
1:G:15:LEU:O	1:G:18:THR:OG1	2.29	0.48
1:C:75:PRO:HG2	1:C:136:ARG:HH12	1.78	0.48
1:A:28:VAL:HG11	1:A:146:ILE:HD11	1.96	0.48
1:C:150:VAL:HB	1:C:151:TYR:CD1	2.49	0.48
1:H:192:ILE:HA	1:H:196:VAL:HG12	1.94	0.48
1:L:36:LEU:HD13	1:L:145:LEU:HD21	1.96	0.48
1:E:42:LYS:HE2	1:E:106:GLU:CG	2.44	0.48
1:F:42:LYS:HD3	1:F:104:ASP:HB3	1.96	0.48
1:A:183:GLU:HG2	1:B:183:GLU:HG2	1.95	0.48
1:J:13:ILE:HD12	1:J:57:GLU:HB2	1.95	0.48
1:I:8:ILE:HA	1:I:47:PHE:O	2.14	0.47
1:K:79:THR:HB	1:K:122:LYS:HD3	1.96	0.47
1:L:163:ALA:HB1	1:L:168:ILE:HB	1.95	0.47
1:J:107:ILE:HD12	1:J:107:ILE:H	1.78	0.47
1:K:86:ASP:CG	1:K:88:ILE:HG22	2.40	0.47
1:D:152:ALA:HA	1:D:156:ILE:HB	1.95	0.47
1:A:9:ALA:O	2:A:303:HOH:O	2.20	0.47
1:E:65:LEU:HD11	1:E:205:LEU:HD23	1.96	0.47
1:E:190:LYS:HD2	1:E:194:GLU:HG3	1.97	0.47
1:F:42:LYS:HD3	1:F:104:ASP:CG	2.39	0.47
1:H:23:LYS:N	2:H:306:HOH:O	2.47	0.47
1:J:107:ILE:HD11	1:J:119:GLN:OE1	2.15	0.47
1:K:73:ASN:C	1:K:73:ASN:HD22	2.23	0.47
1:J:168:ILE:O	1:J:170:PRO:HD3	2.14	0.47
1:I:152:ALA:HA	1:I:156:ILE:HB	1.96	0.46
1:F:20:PRO:HB2	1:F:193:THR:HG21	1.97	0.46
1:L:20:PRO:HB2	1:L:193:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LYS:CE	1:B:70:ARG:HH21	2.26	0.46
1:B:83:PRO:HD3	1:B:105:THR:HG21	1.98	0.46
1:D:106:GLU:CD	1:D:106:GLU:H	2.23	0.46
1:I:136:ARG:CG	2:I:327:HOH:O	2.64	0.46
1:J:38:HIS:HA	1:J:79:THR:OG1	2.15	0.46
1:J:94:THR:HG22	1:J:98:GLY:O	2.15	0.46
1:H:69:ALA:HB1	1:H:74:ILE:HB	1.97	0.46
1:L:185:HIS:O	1:L:189:LEU:HG	2.16	0.46
1:G:64:GLU:O	1:G:68:LEU:HD13	2.16	0.46
1:A:164:PHE:HB2	1:A:196:VAL:HG23	1.96	0.46
1:B:70:ARG:HH22	1:B:114:GLU:CG	2.29	0.46
1:D:66:LYS:CE	1:D:70:ARG:NH2	2.77	0.46
1:D:190:LYS:O	1:D:193:THR:HG22	2.14	0.46
1:F:200:THR:OG1	1:F:201:SER:N	2.48	0.46
1:G:85:GLN:HG2	1:G:123:TRP:CH2	2.50	0.46
1:G:190:LYS:O	1:G:193:THR:HG22	2.16	0.46
1:K:55:VAL:HB	1:K:56:PRO:HD3	1.97	0.46
1:K:126:SER:OG	1:K:162:ASP:OD2	2.30	0.46
1:A:187:HIS:CE1	1:F:187:HIS:NE2	2.84	0.46
1:A:192:ILE:HA	1:A:196:VAL:HG12	1.97	0.46
1:G:26:TRP:CZ3	1:G:170:PRO:HD2	2.50	0.46
1:F:42:LYS:HD3	1:F:104:ASP:CB	2.45	0.46
1:H:65:LEU:HD12	1:H:65:LEU:HA	1.56	0.45
1:H:152:ALA:HA	1:H:156:ILE:HG13	1.98	0.45
1:D:66:LYS:HE2	1:D:70:ARG:CZ	2.46	0.45
1:D:85:GLN:HG2	1:D:123:TRP:CZ3	2.51	0.45
1:K:73:ASN:O	1:K:73:ASN:ND2	2.49	0.45
1:C:136:ARG:CZ	1:C:140:THR:HG21	2.46	0.45
1:L:89:GLU:OE2	1:L:123:TRP:CD1	2.69	0.45
1:C:36:LEU:HD11	1:C:79:THR:HG23	1.98	0.45
1:D:38:HIS:CE1	1:D:155:GLY:HA3	2.52	0.45
1:D:65:LEU:HA	1:D:65:LEU:HD12	1.78	0.45
1:G:165:MET:HG2	1:H:124:ARG:HB3	1.97	0.45
1:G:52:GLN:HA	1:G:52:GLN:OE1	2.17	0.45
1:K:136:ARG:HD3	1:L:136:ARG:HH12	1.81	0.45
1:L:107:ILE:HD12	1:L:107:ILE:H	1.81	0.45
1:D:79:THR:HB	1:D:122:LYS:HD3	1.99	0.45
1:L:150:VAL:HG12	1:L:178:ALA:HB3	1.98	0.45
1:A:164:PHE:CB	1:A:196:VAL:HG23	2.46	0.45
1:A:183:GLU:HG3	1:B:183:GLU:HG3	1.99	0.45
1:K:42:LYS:HD3	1:K:108:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASP:HA	1:B:106:GLU:OE2	2.16	0.44
1:D:85:GLN:HG2	1:D:123:TRP:CH2	2.52	0.44
1:H:136:ARG:NE	1:H:140:THR:HG21	2.31	0.44
1:B:55:VAL:O	1:B:59:LEU:HG	2.17	0.44
1:I:147:ILE:HG22	1:I:156:ILE:HD12	1.98	0.44
1:K:42:LYS:NZ	1:K:109:SER:H	2.15	0.44
1:K:123:TRP:O	1:K:124:ARG:HD3	2.16	0.44
1:C:61:ASN:O	1:C:65:LEU:HB2	2.18	0.44
1:D:136:ARG:HD2	1:E:86:ASP:OD1	2.16	0.44
1:E:168:ILE:O	1:E:170:PRO:HD3	2.18	0.44
1:K:20:PRO:HB2	1:K:193:THR:HG21	1.99	0.44
1:L:82:PRO:O	1:L:85:GLN:NE2	2.49	0.44
1:K:65:LEU:HD21	1:K:205:LEU:HD23	1.98	0.44
1:A:66:LYS:CE	1:A:70:ARG:HH21	2.31	0.44
1:J:185:HIS:O	1:J:189:LEU:HG	2.18	0.44
1:J:38:HIS:CE1	1:J:155:GLY:HA3	2.53	0.44
1:K:50:HIS:N	2:K:307:HOH:O	2.50	0.44
1:L:36:LEU:CD2	1:L:38:HIS:HB2	2.48	0.44
1:B:79:THR:HB	1:B:122:LYS:HD2	2.00	0.43
1:D:36:LEU:HD11	1:D:79:THR:HG23	2.00	0.43
1:K:8:ILE:HA	1:K:47:PHE:O	2.18	0.43
1:L:38:HIS:CE1	1:L:155:GLY:HA3	2.53	0.43
1:F:36:LEU:HB2	1:F:145:LEU:HD11	2.00	0.43
1:H:64:GLU:O	1:H:68:LEU:HD13	2.18	0.43
1:F:177:VAL:O	1:F:185:HIS:HE1	2.02	0.43
1:G:187:HIS:ND1	1:H:187:HIS:CE1	2.86	0.43
1:H:58:LEU:O	1:H:62:ILE:HG13	2.19	0.43
1:L:90:ARG:HG2	1:L:94:THR:HG23	1.99	0.43
1:D:26:TRP:CZ3	1:D:170:PRO:HD2	2.54	0.43
1:K:50:HIS:HA	1:K:55:VAL:HG11	2.00	0.43
1:A:49:ASP:OD1	1:A:51:SER:OG	2.36	0.43
1:F:152:ALA:HB3	1:F:179:ASP:OD2	2.19	0.43
1:L:38:HIS:HA	1:L:79:THR:OG1	2.18	0.43
1:A:118:ILE:HD12	1:H:86:ASP:HA	2.01	0.43
1:A:152:ALA:HA	1:A:156:ILE:HB	2.01	0.43
1:D:42:LYS:HE3	1:D:108:VAL:HA	2.00	0.43
1:G:187:HIS:HD2	1:G:188:THR:H	1.66	0.43
1:K:90:ARG:NH2	1:K:97:TRP:HB2	2.34	0.43
1:A:67:SER:O	1:A:71:GLN:HG3	2.19	0.43
1:B:194:GLU:HG3	1:B:195:ARG:CZ	2.49	0.43
1:J:55:VAL:HB	1:J:56:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:LEU:HD21	1:L:38:HIS:HB2	2.01	0.43
1:J:144:GLN:HB3	1:J:171:PHE:HE1	1.84	0.42
1:G:164:PHE:HB2	1:G:196:VAL:HG23	2.00	0.42
1:B:39:ASP:OD1	1:B:122:LYS:HD3	2.20	0.42
1:H:65:LEU:HD11	1:H:205:LEU:HD22	2.02	0.42
1:J:20:PRO:HB2	1:J:193:THR:HG21	2.02	0.42
1:J:36:LEU:HB2	1:J:145:LEU:HD11	2.00	0.42
1:K:192:ILE:HA	1:K:196:VAL:HG13	2.01	0.42
1:K:103:LYS:HG2	1:K:104:ASP:N	2.34	0.42
1:L:15:LEU:O	1:L:18:THR:OG1	2.37	0.42
1:H:41:GLN:NE2	1:H:80:ALA:HB1	2.35	0.42
1:I:86:ASP:OD1	1:I:88:ILE:HD12	2.19	0.42
1:K:172:VAL:HG21	1:K:192:ILE:HG13	2.01	0.42
1:H:24:VAL:HG22	2:H:306:HOH:O	2.19	0.42
1:L:70:ARG:NH1	1:L:73:ASN:HA	2.35	0.42
1:I:190:LYS:HE3	1:I:194:GLU:CD	2.45	0.42
1:D:122:LYS:HE2	1:D:124:ARG:O	2.20	0.41
1:F:38:HIS:CE1	1:F:155:GLY:HA3	2.55	0.41
1:J:70:ARG:NH2	1:J:117:ASP:OD2	2.49	0.41
1:B:8:ILE:HA	1:B:47:PHE:O	2.20	0.41
1:E:122:LYS:HE2	1:E:124:ARG:O	2.20	0.41
1:L:183:GLU:OE1	1:L:183:GLU:N	2.49	0.41
1:J:38:HIS:NE2	1:J:122:LYS:HE3	2.35	0.41
1:D:140:THR:HG22	1:D:140:THR:O	2.20	0.41
1:H:38:HIS:CE1	1:H:155:GLY:HA3	2.55	0.41
1:H:106:GLU:H	1:H:106:GLU:CD	2.28	0.41
1:L:55:VAL:HB	1:L:56:PRO:HD3	2.02	0.41
1:L:64:GLU:O	1:L:68:LEU:HG	2.21	0.41
1:G:45:ILE:HG13	1:G:108:VAL:HG11	2.02	0.41
1:G:106:GLU:CD	1:G:106:GLU:H	2.28	0.41
1:G:187:HIS:HD2	1:G:188:THR:N	2.18	0.41
1:F:118:ILE:HD13	1:F:136:ARG:HH21	1.85	0.41
1:C:21:LYS:HE2	1:C:21:LYS:HB2	1.64	0.41
1:C:65:LEU:HA	1:C:65:LEU:HD12	1.72	0.41
1:F:8:ILE:HA	1:F:47:PHE:O	2.21	0.41
1:F:123:TRP:O	1:F:124:ARG:HD3	2.20	0.41
1:J:124:ARG:CZ	1:J:130:LYS:HE3	2.50	0.41
1:B:140:THR:HG23	1:B:142:ARG:HB2	2.03	0.41
1:E:38:HIS:NE2	1:E:122:LYS:HE3	2.36	0.41
1:F:86:ASP:CG	1:F:88:ILE:HG22	2.46	0.41
1:A:85:GLN:OE1	1:A:90:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:HG2	1:B:183:GLU:CG	2.50	0.41
1:B:57:GLU:H	1:B:57:GLU:CD	2.27	0.41
1:B:150:VAL:HB	1:B:151:TYR:CD1	2.56	0.41
1:B:168:ILE:O	1:B:170:PRO:HD3	2.21	0.41
1:F:94:THR:HA	1:F:98:GLY:O	2.20	0.41
1:I:50:HIS:CD2	1:I:50:HIS:H	2.37	0.41
1:L:70:ARG:NE	1:L:70:ARG:HA	2.35	0.41
1:A:110:GLU:OE1	1:A:110:GLU:N	2.45	0.41
1:E:33:ALA:O	1:E:74:ILE:HG23	2.21	0.41
1:A:50:HIS:CD2	1:A:50:HIS:H	2.39	0.40
1:C:152:ALA:HA	1:C:156:ILE:HG13	2.03	0.40
1:D:112:SER:HA	1:D:113:PRO:HD3	1.93	0.40
1:G:33:ALA:HA	1:G:144:GLN:HB2	2.03	0.40
1:J:85:GLN:HB3	1:J:90:ARG:HB2	2.02	0.40
1:F:112:SER:HA	1:F:113:PRO:HD3	1.98	0.40
1:L:28:VAL:HG11	1:L:146:ILE:HD11	2.02	0.40
1:A:39:ASP:OD1	1:A:122:LYS:HD3	2.20	0.40
1:H:150:VAL:HB	1:H:151:TYR:CD1	2.57	0.40
1:G:164:PHE:CB	1:G:196:VAL:HG23	2.52	0.40
1:J:150:VAL:HA	1:J:151:TYR:HA	1.93	0.40
1:A:65:LEU:HD21	1:A:205:LEU:HD23	2.04	0.40
1:D:103:LYS:HG2	2:D:309:HOH:O	2.21	0.40
1:I:149:GLY:O	1:I:177:VAL:HA	2.21	0.40
1:K:66:LYS:NZ	1:K:117:ASP:OD2	2.50	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:324:HOH:O	2:J:312:HOH:O[1_455]	2.00	0.20
2:A:333:HOH:O	2:H:330:HOH:O[1_655]	2.06	0.14
1:A:73:ASN:ND2	1:H:70:ARG:NH1[1_655]	2.09	0.11
1:D:12:SER:OG	1:J:71:GLN:NE2[2_656]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	196/217 (90%)	184 (94%)	11 (6%)	1 (0%)	24	31
1	B	196/217 (90%)	186 (95%)	9 (5%)	1 (0%)	24	31
1	C	196/217 (90%)	189 (96%)	6 (3%)	1 (0%)	24	31
1	D	196/217 (90%)	188 (96%)	8 (4%)	0	100	100
1	E	196/217 (90%)	186 (95%)	9 (5%)	1 (0%)	24	31
1	F	196/217 (90%)	188 (96%)	7 (4%)	1 (0%)	24	31
1	G	196/217 (90%)	188 (96%)	7 (4%)	1 (0%)	24	31
1	H	196/217 (90%)	187 (95%)	8 (4%)	1 (0%)	24	31
1	I	196/217 (90%)	185 (94%)	11 (6%)	0	100	100
1	J	196/217 (90%)	185 (94%)	9 (5%)	2 (1%)	12	15
1	K	196/217 (90%)	187 (95%)	8 (4%)	1 (0%)	24	31
1	L	196/217 (90%)	185 (94%)	9 (5%)	2 (1%)	12	15
All	All	2352/2604 (90%)	2238 (95%)	102 (4%)	12 (0%)	24	31

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	115	ASP
1	F	115	ASP
1	H	115	ASP
1	J	115	ASP
1	K	115	ASP
1	J	84	ASN
1	L	101	LEU
1	A	115	ASP
1	B	115	ASP
1	E	115	ASP
1	L	115	ASP
1	G	154	ILE

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	170/192 (88%)	170 (100%)	0	100	100
1	B	170/192 (88%)	169 (99%)	1 (1%)	78	89
1	C	170/192 (88%)	170 (100%)	0	100	100
1	D	170/192 (88%)	167 (98%)	3 (2%)	51	70
1	E	170/192 (88%)	170 (100%)	0	100	100
1	F	170/192 (88%)	168 (99%)	2 (1%)	63	79
1	G	170/192 (88%)	168 (99%)	2 (1%)	63	79
1	H	170/192 (88%)	170 (100%)	0	100	100
1	I	170/192 (88%)	169 (99%)	1 (1%)	78	89
1	J	170/192 (88%)	169 (99%)	1 (1%)	78	89
1	K	170/192 (88%)	169 (99%)	1 (1%)	78	89
1	L	170/192 (88%)	169 (99%)	1 (1%)	78	89
All	All	2040/2304 (88%)	2028 (99%)	12 (1%)	78	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	196	VAL
1	D	63	SER
1	D	136	ARG
1	D	196	VAL
1	F	63	SER
1	F	196	VAL
1	G	63	SER
1	G	136	ARG
1	I	63	SER
1	J	196	VAL
1	K	196	VAL
1	L	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN

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Mol	Chain	Res	Type
1	A	187	HIS
1	B	187	HIS
1	C	27	HIS
1	D	52	GLN
1	E	71	GLN
1	E	84	ASN
1	E	169	GLN
1	F	27	HIS
1	F	29	GLN
1	F	71	GLN
1	F	85	GLN
1	H	27	HIS
1	H	71	GLN
1	H	186	HIS
1	I	29	GLN
1	I	41	GLN
1	I	50	HIS
1	I	71	GLN
1	I	186	HIS
1	J	27	HIS
1	J	71	GLN
1	J	141	GLN
1	K	29	GLN
1	K	50	HIS
1	K	71	GLN
1	K	73	ASN
1	L	27	HIS
1	L	29	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	198/217 (91%)	-1.14	0 100 100	28, 42, 64, 73	0
1	B	198/217 (91%)	-1.18	0 100 100	30, 42, 65, 73	0
1	C	198/217 (91%)	-1.01	0 100 100	29, 52, 75, 92	0
1	D	198/217 (91%)	-1.17	0 100 100	29, 43, 64, 75	0
1	E	198/217 (91%)	-1.08	0 100 100	32, 47, 71, 91	0
1	F	198/217 (91%)	-1.01	0 100 100	31, 53, 78, 93	0
1	G	198/217 (91%)	-1.17	0 100 100	28, 43, 64, 74	0
1	H	198/217 (91%)	-0.99	0 100 100	27, 54, 75, 97	0
1	I	198/217 (91%)	-1.15	0 100 100	31, 47, 69, 91	0
1	J	198/217 (91%)	-0.87	0 100 100	33, 61, 89, 113	0
1	K	198/217 (91%)	-0.96	0 100 100	31, 54, 80, 91	0
1	L	198/217 (91%)	-0.93	0 100 100	34, 60, 87, 107	0
All	All	2376/2604 (91%)	-1.05	0 100 100	27, 49, 77, 113	0

There are no RSRZ outliers to report.

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.