



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:17 AM GMT

PDB ID : 4LDB
Title : Crystal Structure of Ebola Virus VP40 Dimer
Authors : Bornholdt, Z.A.; Ableson, D.M.; Saphire, E.O.
Deposited on : 2013-06-24
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

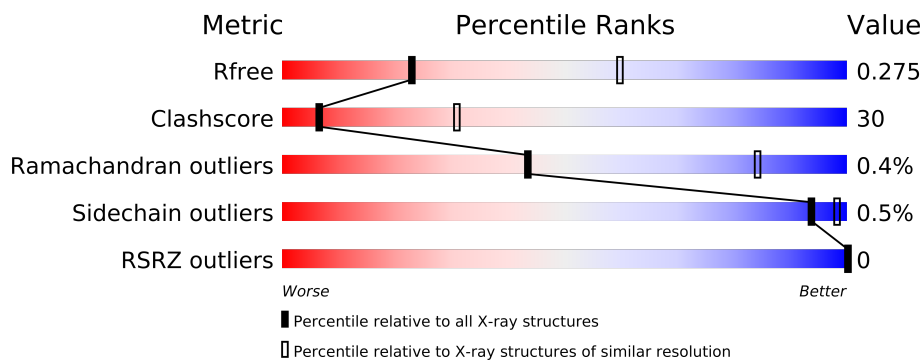
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	297	
1	B	297	
1	C	297	
1	D	297	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7574 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Matrix protein VP40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2027	1309	338	372	8			
1	B	249	Total	C	N	O	S	0	0	0
			1912	1239	319	346	8			
1	C	237	Total	C	N	O	S	0	0	0
			1824	1189	302	326	7			
1	D	235	Total	C	N	O	S	0	0	0
			1811	1175	300	328	8			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP Q05128
A	31	ALA	-	EXPRESSION TAG	UNP Q05128
A	32	HIS	-	EXPRESSION TAG	UNP Q05128
A	33	HIS	-	EXPRESSION TAG	UNP Q05128
A	34	HIS	-	EXPRESSION TAG	UNP Q05128
A	35	HIS	-	EXPRESSION TAG	UNP Q05128
A	36	HIS	-	EXPRESSION TAG	UNP Q05128
A	37	HIS	-	EXPRESSION TAG	UNP Q05128
A	38	VAL	-	EXPRESSION TAG	UNP Q05128
A	39	ASP	-	EXPRESSION TAG	UNP Q05128
A	40	ASP	-	EXPRESSION TAG	UNP Q05128
A	41	ASP	-	EXPRESSION TAG	UNP Q05128
A	42	ASP	-	EXPRESSION TAG	UNP Q05128
A	43	LYS	-	EXPRESSION TAG	UNP Q05128
B	30	MET	-	EXPRESSION TAG	UNP Q05128
B	31	ALA	-	EXPRESSION TAG	UNP Q05128
B	32	HIS	-	EXPRESSION TAG	UNP Q05128
B	33	HIS	-	EXPRESSION TAG	UNP Q05128
B	34	HIS	-	EXPRESSION TAG	UNP Q05128
B	35	HIS	-	EXPRESSION TAG	UNP Q05128
B	36	HIS	-	EXPRESSION TAG	UNP Q05128

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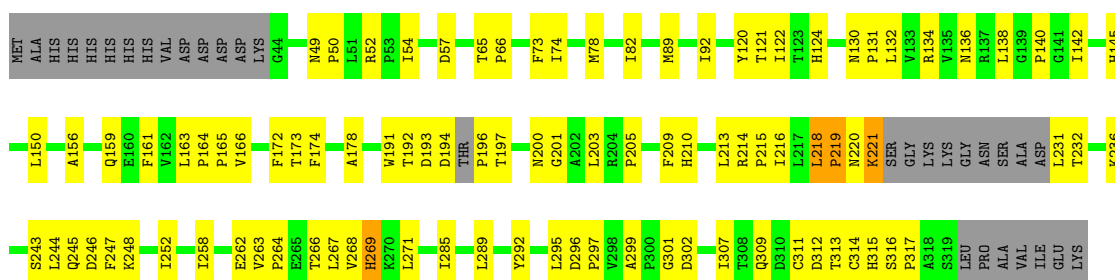
Chain	Residue	Modelled	Actual	Comment	Reference
B	37	HIS	-	EXPRESSION TAG	UNP Q05128
B	38	VAL	-	EXPRESSION TAG	UNP Q05128
B	39	ASP	-	EXPRESSION TAG	UNP Q05128
B	40	ASP	-	EXPRESSION TAG	UNP Q05128
B	41	ASP	-	EXPRESSION TAG	UNP Q05128
B	42	ASP	-	EXPRESSION TAG	UNP Q05128
B	43	LYS	-	EXPRESSION TAG	UNP Q05128
C	30	MET	-	EXPRESSION TAG	UNP Q05128
C	31	ALA	-	EXPRESSION TAG	UNP Q05128
C	32	HIS	-	EXPRESSION TAG	UNP Q05128
C	33	HIS	-	EXPRESSION TAG	UNP Q05128
C	34	HIS	-	EXPRESSION TAG	UNP Q05128
C	35	HIS	-	EXPRESSION TAG	UNP Q05128
C	36	HIS	-	EXPRESSION TAG	UNP Q05128
C	37	HIS	-	EXPRESSION TAG	UNP Q05128
C	38	VAL	-	EXPRESSION TAG	UNP Q05128
C	39	ASP	-	EXPRESSION TAG	UNP Q05128
C	40	ASP	-	EXPRESSION TAG	UNP Q05128
C	41	ASP	-	EXPRESSION TAG	UNP Q05128
C	42	ASP	-	EXPRESSION TAG	UNP Q05128
C	43	LYS	-	EXPRESSION TAG	UNP Q05128
D	30	MET	-	EXPRESSION TAG	UNP Q05128
D	31	ALA	-	EXPRESSION TAG	UNP Q05128
D	32	HIS	-	EXPRESSION TAG	UNP Q05128
D	33	HIS	-	EXPRESSION TAG	UNP Q05128
D	34	HIS	-	EXPRESSION TAG	UNP Q05128
D	35	HIS	-	EXPRESSION TAG	UNP Q05128
D	36	HIS	-	EXPRESSION TAG	UNP Q05128
D	37	HIS	-	EXPRESSION TAG	UNP Q05128
D	38	VAL	-	EXPRESSION TAG	UNP Q05128
D	39	ASP	-	EXPRESSION TAG	UNP Q05128
D	40	ASP	-	EXPRESSION TAG	UNP Q05128
D	41	ASP	-	EXPRESSION TAG	UNP Q05128
D	42	ASP	-	EXPRESSION TAG	UNP Q05128
D	43	LYS	-	EXPRESSION TAG	UNP Q05128

3 Residue-property plots

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

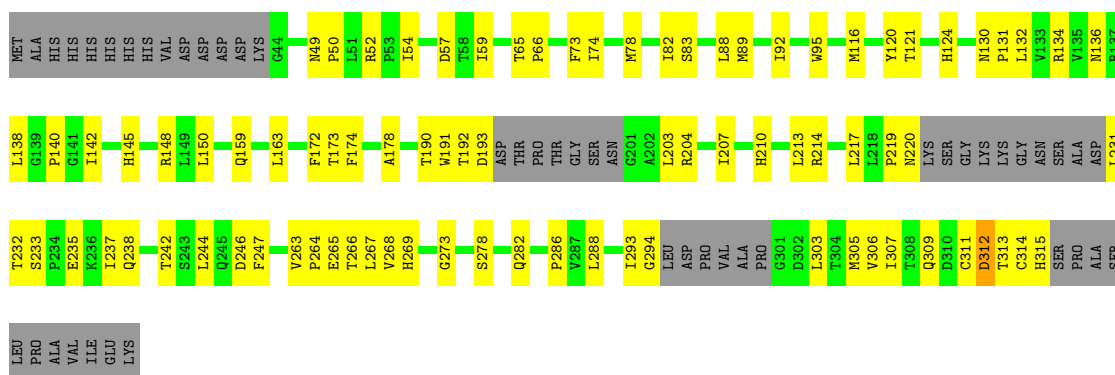
- Molecule 1: Matrix protein VP40

Chain A:



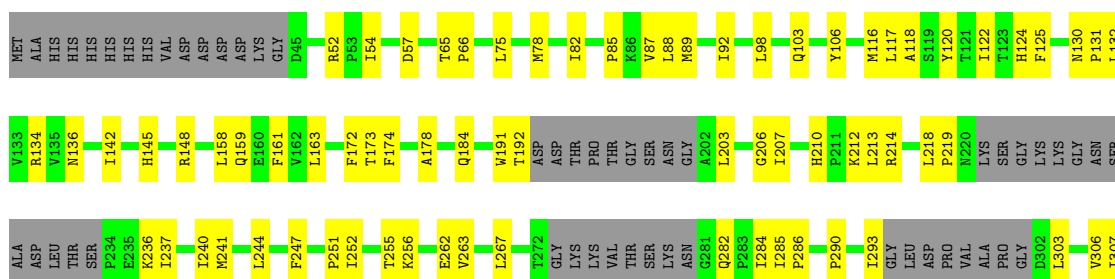
- Molecule 1: Matrix protein VP40

Chain B:



- Molecule 1: Matrix protein VP40

Chain C:



T308	GLN
	ASP
	CYS
D312	
T313	
C314	
H315	
A318	ASP
S319	
L320	
P321	
A322	VAL
	ILE
	GLU
	LYS

● Molecule 1: Matrix protein VP40

Chain D:

MET	
ALA	
HIS	
HIS	
HIS	
HIS	
HIS	
HIS	
VAL	
ASP	
ASP	
ASP	
LYS	
GLY	D45
R52	
P63	
I54	
	D57
D60	
T65	P66
L75	
M78	
I82	
SER	GLY
GLY	
PRO	
LYS	
VAL	
LEU	
	M89
I92	
	P93
I94	
	P95
	L96
	P97
	L98
Q103	
Y106	
A118	
	S119
	Y120
H124	
N130	

P131	
L132	
V133	
R134	
	V135
	M136
I142	
H145	
R148	
	L149
	L150
F157	
	L158
	Q159
L163	
P164	
	P165
F172	
T173	
F174	
A178	
Q184	
	P185
W191	
T192	
ASP	
GLY	
PRO	
LYS	
THR	
PRO	
THR	
GLY	
SER	
ASN	
	G201
	A202
	L203
	R204
	P205
	G206
	I207
H210	
	P211
	K212
	L213
	R214
L218	
	P219
	N220
	LYS

SER	
GLY	
LYS	
LYS	
GLY	
ASN	
SER	
ALA	
ASP	
LEU	T232
	S233
K236	
I237	
	I240
	M241
L244	
	P251
K256	
	E262
E265	
T266	
L267	
V268	
H269	
LYS	
LEU	
THR	
GLY	
LYS	
LYS	
VAL	
THR	
SER	
LYS	
	N280
	G281
	Q282
	L288
	L289
	P290
T293	
GLY	
LEU	
ASP	
PRO	
VAL	
ALA	
PRO	G301
	D302

L303	
V306	
I307	
T308	
Q309	
D310	
C311	
T313	
C314	
H315	
A318	
S319	
L320	
P321	
ALA	
VAL	
ILE	
GLU	
LYS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	160.00Å 160.00Å 89.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.10 45.23 – 2.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-3.10) 83.1 (45.23-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.245 , 0.282 0.245 , 0.275	Depositor DCC
R_{free} test set	1219 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	EDS
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 50277 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7574	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.46	0/2079	0.47	0/2845
1	B	0.44	0/1959	0.43	0/2677
1	C	0.42	0/1871	0.43	0/2560
1	D	0.40	0/1857	0.41	0/2542
All	All	0.43	0/7766	0.44	0/10624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2027	0	2095	149	0
1	B	1912	0	1983	134	0
1	C	1824	0	1886	102	0
1	D	1811	0	1858	107	0
All	All	7574	0	7822	456	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (456) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:156:ALA:HB3	1:A:315:HIS:CE1	1.55	1.41
1:A:156:ALA:HB3	1:A:315:HIS:NE2	1.38	1.33
1:D:204:ARG:CD	1:D:311:CYS:HB2	1.67	1.25
1:A:89:MET:CB	1:A:92:ILE:HD11	1.71	1.19
1:A:315:HIS:CD2	1:A:316:SER:H	1.58	1.19
1:D:89:MET:CB	1:D:92:ILE:HD11	1.73	1.18
1:B:231:LEU:CD2	1:B:232:THR:H	1.58	1.16
1:B:231:LEU:HD23	1:B:232:THR:N	1.59	1.15
1:D:89:MET:HB3	1:D:92:ILE:HD11	1.18	1.14
1:D:204:ARG:HD2	1:D:311:CYS:HB2	1.27	1.13
1:C:89:MET:CB	1:C:92:ILE:HD11	1.78	1.13
1:C:89:MET:HB3	1:C:92:ILE:HD11	1.13	1.13
1:A:315:HIS:CG	1:A:317:PRO:HD2	1.84	1.12
1:B:89:MET:HB3	1:B:92:ILE:HD11	1.19	1.11
1:A:89:MET:HB3	1:A:92:ILE:HD11	1.15	1.10
1:D:124:HIS:CE1	1:D:172:PHE:CE1	2.39	1.10
1:A:124:HIS:CE1	1:A:172:PHE:CE1	2.39	1.10
1:A:138:LEU:HD13	1:B:138:LEU:HD13	1.29	1.07
1:A:138:LEU:HD13	1:B:138:LEU:CD1	1.85	1.06
1:A:138:LEU:CD1	1:B:138:LEU:HD13	1.85	1.05
1:A:156:ALA:CB	1:A:315:HIS:CE1	2.39	1.04
1:B:89:MET:CB	1:B:92:ILE:HD11	1.86	1.04
1:A:231:LEU:O	1:A:236:LYS:HD3	1.59	1.03
1:A:140:PRO:HD3	1:B:140:PRO:HD3	1.38	1.01
1:B:207:ILE:HG23	1:B:303:LEU:HD13	1.41	1.01
1:C:134:ARG:CZ	1:C:136:ASN:HD21	1.76	0.98
1:B:263:VAL:HG23	1:B:268:VAL:CG1	1.94	0.98
1:A:315:HIS:CD2	1:A:317:PRO:HD2	2.00	0.96
1:D:204:ARG:HD3	1:D:311:CYS:HB2	1.45	0.95
1:B:124:HIS:CE1	1:B:172:PHE:CE2	2.54	0.95
1:B:207:ILE:CG2	1:B:303:LEU:HD13	1.97	0.95
1:A:205:PRO:HD3	1:A:232:THR:HG22	1.49	0.94
1:B:210:HIS:HB3	1:B:213:LEU:HB2	1.50	0.93
1:C:210:HIS:HE1	1:C:212:LYS:HB2	1.33	0.92
1:D:204:ARG:CD	1:D:311:CYS:CB	2.47	0.92
1:A:156:ALA:CB	1:A:315:HIS:NE2	2.32	0.91
1:B:231:LEU:HD23	1:B:232:THR:H	0.78	0.91
1:D:265:GLU:O	1:D:268:VAL:HG12	1.70	0.91
1:A:315:HIS:CD2	1:A:316:SER:N	2.39	0.91
1:D:204:ARG:HD3	1:D:311:CYS:CB	1.99	0.91
1:A:89:MET:CB	1:A:92:ILE:CD1	2.50	0.89
1:B:148:ARG:NH2	1:B:214:ARG:HH12	1.71	0.89
1:A:296:ASP:OD1	1:A:297:PRO:HD2	1.73	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:124:HIS:CE1	1:C:172:PHE:CE2	2.64	0.86
1:C:203:LEU:HD13	1:C:307:ILE:CG2	2.06	0.86
1:A:140:PRO:HG3	1:B:140:PRO:HG3	1.59	0.85
1:B:148:ARG:NH1	1:B:214:ARG:HH22	1.74	0.85
1:A:89:MET:HB2	1:A:92:ILE:CD1	2.08	0.84
1:C:236:LYS:O	1:C:240:ILE:HG22	1.77	0.84
1:D:89:MET:CB	1:D:92:ILE:CD1	2.55	0.83
1:A:315:HIS:CE1	1:A:317:PRO:CD	2.61	0.83
1:D:89:MET:HB2	1:D:92:ILE:HD11	1.61	0.83
1:C:89:MET:CB	1:C:92:ILE:CD1	2.57	0.81
1:D:89:MET:HB2	1:D:92:ILE:CD1	2.11	0.81
1:D:210:HIS:HE1	1:D:212:LYS:HB2	1.47	0.80
1:D:204:ARG:HD2	1:D:311:CYS:CB	2.10	0.80
1:A:315:HIS:HD2	1:A:316:SER:H	1.27	0.80
1:D:203:LEU:HD13	1:D:307:ILE:CG2	2.12	0.79
1:B:311:CYS:SG	1:B:313:THR:O	2.40	0.79
1:A:89:MET:HB2	1:A:92:ILE:HD11	1.65	0.79
1:A:197:THR:HB	1:A:201:GLY:HA2	1.64	0.79
1:B:263:VAL:HG23	1:B:268:VAL:HG13	1.64	0.78
1:B:172:PHE:HE1	1:B:174:PHE:CZ	2.02	0.78
1:A:231:LEU:HD23	1:A:232:THR:N	1.99	0.78
1:C:172:PHE:HE1	1:C:174:PHE:CZ	2.02	0.78
1:D:236:LYS:O	1:D:240:ILE:HG22	1.83	0.77
1:A:231:LEU:N	1:A:236:LYS:HZ2	1.83	0.77
1:C:148:ARG:NH1	1:C:321:PRO:HA	1.99	0.77
1:B:148:ARG:HH12	1:B:214:ARG:HH22	1.31	0.76
1:D:210:HIS:CE1	1:D:212:LYS:HB2	2.21	0.76
1:B:192:THR:O	1:B:193:ASP:HB2	1.86	0.75
1:B:89:MET:CB	1:B:92:ILE:CD1	2.63	0.75
1:A:315:HIS:CG	1:A:317:PRO:CD	2.69	0.74
1:C:210:HIS:CE1	1:C:212:LYS:HB2	2.19	0.74
1:B:148:ARG:HH22	1:B:214:ARG:HH12	1.33	0.74
1:A:156:ALA:CB	1:A:315:HIS:HE1	2.01	0.73
1:B:124:HIS:CG	1:B:172:PHE:CZ	2.75	0.73
1:D:148:ARG:NH1	1:D:321:PRO:HA	2.02	0.73
1:D:184:GLN:OE1	1:D:256:LYS:NZ	2.21	0.73
1:A:124:HIS:CG	1:A:172:PHE:CZ	2.77	0.72
1:D:82:ILE:HB	1:D:173:THR:CG2	2.19	0.72
1:A:54:ILE:HG12	1:D:54:ILE:HG12	1.72	0.72
1:A:205:PRO:CD	1:A:232:THR:HG22	2.20	0.72
1:B:265:GLU:HA	1:B:268:VAL:CG2	2.21	0.71
1:D:237:ILE:HA	1:D:240:ILE:CG2	2.20	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:210:HIS:HE1	1:C:212:LYS:CB	2.04	0.71
1:A:89:MET:HB3	1:A:92:ILE:CD1	2.09	0.71
1:A:50:PRO:HG3	1:B:121:THR:HG21	1.73	0.71
1:C:124:HIS:CG	1:C:172:PHE:CZ	2.78	0.71
1:B:266:THR:HG23	1:B:267:LEU:N	2.06	0.71
1:A:203:LEU:HD12	1:A:203:LEU:O	1.92	0.70
1:A:209:PHE:CD1	1:A:295:LEU:HD21	2.27	0.70
1:A:267:LEU:O	1:A:271:LEU:HD23	1.91	0.70
1:A:121:THR:HG21	1:B:50:PRO:HG3	1.74	0.69
1:D:313:THR:O	1:D:313:THR:HG22	1.91	0.69
1:C:89:MET:HB2	1:C:92:ILE:CD1	2.21	0.69
1:A:316:SER:N	1:A:317:PRO:HD2	2.07	0.69
1:A:220:ASN:O	1:A:221:LYS:CB	2.40	0.69
1:A:311:CYS:SG	1:A:313:THR:O	2.51	0.69
1:B:263:VAL:CG2	1:B:268:VAL:CG1	2.71	0.68
1:D:82:ILE:HB	1:D:173:THR:HG22	1.74	0.68
1:D:124:HIS:ND1	1:D:172:PHE:CE1	2.61	0.68
1:B:82:ILE:HB	1:B:173:THR:CG2	2.23	0.68
1:D:124:HIS:CG	1:D:172:PHE:CZ	2.82	0.68
1:C:134:ARG:NH2	1:C:136:ASN:HD21	1.90	0.68
1:C:237:ILE:HA	1:C:240:ILE:CG2	2.24	0.68
1:C:184:GLN:OE1	1:C:256:LYS:NZ	2.27	0.68
1:A:54:ILE:HD11	1:D:54:ILE:HD11	1.76	0.68
1:A:124:HIS:ND1	1:A:172:PHE:CE1	2.62	0.68
1:A:315:HIS:CE1	1:A:317:PRO:HD3	2.28	0.67
1:B:82:ILE:HB	1:B:173:THR:HG22	1.76	0.67
1:A:315:HIS:ND1	1:A:317:PRO:CD	2.58	0.67
1:A:315:HIS:ND1	1:A:317:PRO:CG	2.57	0.67
1:A:220:ASN:O	1:A:221:LYS:HB3	1.94	0.67
1:C:262:GLU:HG3	1:C:282:GLN:HG2	1.77	0.67
1:C:82:ILE:HB	1:C:173:THR:CG2	2.25	0.67
1:D:262:GLU:HG3	1:D:282:GLN:HG2	1.77	0.66
1:B:54:ILE:HG12	1:C:54:ILE:HG12	1.78	0.66
1:A:82:ILE:HB	1:A:173:THR:CG2	2.26	0.66
1:A:220:ASN:C	1:A:220:ASN:OD1	2.34	0.66
1:C:134:ARG:CZ	1:C:136:ASN:ND2	2.56	0.66
1:C:88:LEU:HD12	1:C:88:LEU:N	2.09	0.66
1:A:220:ASN:OD1	1:A:221:LYS:N	2.30	0.65
1:A:309:GLN:HG2	1:C:251:PRO:CG	2.26	0.65
1:D:204:ARG:HH11	1:D:311:CYS:HB2	1.62	0.65
1:A:138:LEU:HD13	1:B:138:LEU:HD12	1.74	0.65
1:B:142:ILE:HG22	1:B:145:HIS:HB2	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:142:ILE:HG22	1:C:145:HIS:HB2	1.78	0.65
1:C:313:THR:O	1:C:313:THR:HG22	1.97	0.65
1:B:89:MET:HB2	1:B:92:ILE:CD1	2.27	0.64
1:A:193:ASP:O	1:A:194:ASP:HB2	1.96	0.64
1:A:209:PHE:CZ	1:A:289:LEU:HD21	2.33	0.64
1:A:315:HIS:CD2	1:A:317:PRO:CD	2.77	0.64
1:C:210:HIS:CE1	1:C:212:LYS:CB	2.80	0.64
1:B:263:VAL:O	1:B:282:GLN:NE2	2.31	0.63
1:C:203:LEU:HD13	1:C:307:ILE:HG22	1.79	0.63
1:B:246:ASP:HB2	1:B:264:PRO:CG	2.29	0.63
1:C:134:ARG:NH1	1:C:136:ASN:HD21	1.96	0.63
1:B:124:HIS:ND1	1:B:172:PHE:CE2	2.67	0.62
1:C:82:ILE:HB	1:C:173:THR:HG22	1.81	0.62
1:A:82:ILE:HB	1:A:173:THR:HG22	1.81	0.62
1:A:315:HIS:ND1	1:A:317:PRO:HD2	2.15	0.62
1:A:54:ILE:CG1	1:D:54:ILE:HG12	2.28	0.62
1:A:221:LYS:NZ	1:A:221:LYS:HB3	2.13	0.62
1:A:124:HIS:CD2	1:A:172:PHE:CZ	2.87	0.62
1:D:142:ILE:HG22	1:D:145:HIS:HB2	1.81	0.62
1:A:54:ILE:HG12	1:D:54:ILE:CG1	2.30	0.61
1:C:306:VAL:HG12	1:C:307:ILE:N	2.15	0.61
1:A:218:LEU:O	1:A:219:PRO:C	2.37	0.61
1:A:209:PHE:CE1	1:A:295:LEU:HD21	2.35	0.61
1:C:132:LEU:HD21	1:C:320:LEU:CD1	2.30	0.61
1:A:89:MET:SD	1:A:166:VAL:HG11	2.40	0.61
1:C:52:ARG:HD3	1:C:118:ALA:O	2.01	0.61
1:D:306:VAL:CG1	1:D:307:ILE:N	2.63	0.60
1:D:203:LEU:HB3	1:D:309:GLN:HA	1.83	0.60
1:B:54:ILE:CG1	1:C:54:ILE:HG12	2.31	0.60
1:A:231:LEU:O	1:A:236:LYS:CD	2.44	0.60
1:C:306:VAL:CG1	1:C:307:ILE:N	2.64	0.60
1:D:192:THR:HG22	1:D:315:HIS:CE1	2.36	0.60
1:C:192:THR:HG22	1:C:315:HIS:NE2	2.16	0.60
1:B:265:GLU:HA	1:B:268:VAL:HG22	1.83	0.60
1:D:124:HIS:CE1	1:D:172:PHE:CD1	2.90	0.60
1:C:244:LEU:O	1:C:244:LEU:HD13	2.02	0.59
1:B:54:ILE:HG12	1:C:54:ILE:CG1	2.32	0.59
1:D:306:VAL:HG12	1:D:307:ILE:N	2.15	0.59
1:C:210:HIS:CE1	1:C:212:LYS:H	2.22	0.58
1:A:203:LEU:HD13	1:A:307:ILE:CG2	2.33	0.58
1:B:293:ILE:O	1:B:294:GLY:C	2.42	0.58
1:B:314:CYS:O	1:B:315:HIS:C	2.40	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:192:THR:HG22	1:D:315:HIS:NE2	2.18	0.58
1:D:244:LEU:O	1:D:244:LEU:HD13	2.03	0.58
1:B:191:TRP:O	1:B:192:THR:HG23	2.04	0.58
1:A:205:PRO:HD3	1:A:232:THR:CG2	2.30	0.58
1:C:192:THR:HG22	1:C:315:HIS:CE1	2.39	0.58
1:A:315:HIS:CE1	1:A:317:PRO:HG3	2.39	0.57
1:C:203:LEU:HD12	1:C:203:LEU:O	2.03	0.57
1:B:54:ILE:CG1	1:C:54:ILE:CG1	2.82	0.57
1:D:132:LEU:HD21	1:D:320:LEU:CD1	2.35	0.57
1:A:140:PRO:HD3	1:B:140:PRO:CD	2.23	0.57
1:A:267:LEU:HG	1:A:271:LEU:HD23	1.86	0.57
1:B:145:HIS:CE1	1:B:150:LEU:HD12	2.38	0.57
1:B:306:VAL:HG12	1:B:307:ILE:N	2.19	0.57
1:D:131:PRO:O	1:D:132:LEU:HD12	2.05	0.57
1:A:315:HIS:CE1	1:A:317:PRO:CG	2.88	0.57
1:A:54:ILE:CG1	1:D:54:ILE:CG1	2.83	0.57
1:D:203:LEU:HD13	1:D:307:ILE:HG22	1.83	0.57
1:B:266:THR:HG23	1:B:267:LEU:H	1.69	0.57
1:B:288:LEU:HD12	1:B:288:LEU:N	2.19	0.57
1:A:315:HIS:CG	1:A:316:SER:N	2.73	0.57
1:C:132:LEU:HD21	1:C:320:LEU:HD12	1.87	0.57
1:A:244:LEU:HD12	1:A:244:LEU:O	2.04	0.57
1:D:78:MET:HB3	1:D:178:ALA:HB3	1.87	0.57
1:C:89:MET:HB3	1:C:92:ILE:CD1	2.08	0.56
1:A:210:HIS:HB3	1:A:213:LEU:HB2	1.87	0.56
1:C:131:PRO:O	1:C:132:LEU:HD12	2.04	0.56
1:C:213:LEU:HD11	1:C:293:ILE:CD1	2.35	0.56
1:B:311:CYS:C	1:B:313:THR:H	2.07	0.56
1:A:309:GLN:HG2	1:C:251:PRO:CD	2.36	0.56
1:B:265:GLU:O	1:B:268:VAL:CG2	2.54	0.55
1:A:172:PHE:HE2	1:A:174:PHE:CZ	2.23	0.55
1:A:138:LEU:HD12	1:B:138:LEU:HD13	1.78	0.55
1:B:247:PHE:CE2	1:B:263:VAL:HG12	2.42	0.55
1:B:306:VAL:CG1	1:B:307:ILE:N	2.70	0.55
1:D:210:HIS:CE1	1:D:212:LYS:H	2.24	0.55
1:C:244:LEU:HD13	1:C:244:LEU:C	2.27	0.55
1:C:78:MET:HB3	1:C:178:ALA:HB3	1.89	0.55
1:A:138:LEU:CD1	1:B:138:LEU:CD1	2.63	0.55
1:A:145:HIS:CE1	1:A:150:LEU:HD12	2.42	0.55
1:B:231:LEU:HD23	1:B:232:THR:CA	2.35	0.54
1:C:124:HIS:CD2	1:C:172:PHE:CZ	2.96	0.54
1:C:262:GLU:CG	1:C:282:GLN:HG2	2.37	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:315:HIS:NE2	1:A:317:PRO:CD	2.71	0.54
1:B:219:PRO:O	1:B:220:ASN:C	2.45	0.54
1:B:203:LEU:O	1:B:203:LEU:HD12	2.06	0.54
1:B:246:ASP:C	1:B:264:PRO:HG3	2.28	0.54
1:A:124:HIS:CE1	1:A:172:PHE:CD1	2.95	0.53
1:D:204:ARG:HH11	1:D:311:CYS:CB	2.21	0.53
1:C:124:HIS:ND1	1:C:172:PHE:CE2	2.75	0.53
1:A:243:SER:HB3	1:A:264:PRO:HG2	1.90	0.53
1:C:87:VAL:O	1:C:87:VAL:HG23	2.09	0.53
1:C:134:ARG:NH2	1:C:136:ASN:ND2	2.55	0.53
1:B:124:HIS:CD2	1:B:172:PHE:CZ	2.97	0.53
1:B:311:CYS:O	1:B:313:THR:N	2.41	0.53
1:C:172:PHE:CE1	1:C:174:PHE:CZ	2.92	0.53
1:A:191:TRP:CD2	1:A:219:PRO:HG2	2.43	0.53
1:D:311:CYS:O	1:D:311:CYS:SG	2.66	0.53
1:D:262:GLU:CG	1:D:282:GLN:HG2	2.39	0.53
1:B:78:MET:HB3	1:B:178:ALA:HB3	1.91	0.53
1:B:131:PRO:HB2	1:B:159:GLN:OE1	2.09	0.53
1:A:196:PRO:HG3	1:A:312:ASP:HA	1.91	0.53
1:B:269:HIS:O	1:B:273:GLY:N	2.42	0.52
1:A:267:LEU:HG	1:A:271:LEU:CD2	2.39	0.52
1:A:191:TRP:O	1:A:192:THR:HG23	2.09	0.52
1:A:192:THR:O	1:A:193:ASP:OD1	2.26	0.52
1:A:142:ILE:HG22	1:A:145:HIS:HB2	1.91	0.52
1:C:57:ASP:N	1:C:57:ASP:OD1	2.41	0.52
1:B:54:ILE:HD11	1:C:54:ILE:HD11	1.91	0.52
1:B:263:VAL:CG2	1:B:268:VAL:HG12	2.39	0.52
1:B:265:GLU:CA	1:B:268:VAL:HG22	2.39	0.52
1:D:203:LEU:O	1:D:203:LEU:HD12	2.09	0.52
1:A:309:GLN:HG2	1:C:251:PRO:HG2	1.91	0.52
1:A:299:ALA:O	1:A:302:ASP:CB	2.57	0.52
1:A:315:HIS:NE2	1:A:317:PRO:HD3	2.23	0.52
1:A:159:GLN:HG3	1:A:163:LEU:HD12	1.92	0.52
1:B:124:HIS:CE1	1:B:172:PHE:CD2	2.96	0.52
1:B:315:HIS:O	1:B:315:HIS:CG	2.62	0.52
1:A:124:HIS:CE1	1:A:172:PHE:HE1	2.17	0.52
1:C:125:PHE:HE2	1:C:134:ARG:HE	1.58	0.52
1:B:172:PHE:CE1	1:B:174:PHE:CZ	2.91	0.52
1:C:88:LEU:CD1	1:C:88:LEU:N	2.73	0.52
1:A:78:MET:HB3	1:A:178:ALA:HB3	1.92	0.52
1:A:221:LYS:HZ1	1:A:221:LYS:HB3	1.75	0.52
1:B:57:ASP:OD1	1:B:57:ASP:N	2.38	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:125:PHE:HE2	1:C:134:ARG:NE	2.06	0.51
1:D:244:LEU:C	1:D:244:LEU:HD13	2.30	0.51
1:D:134:ARG:CZ	1:D:136:ASN:HD21	2.23	0.51
1:D:124:HIS:CD2	1:D:172:PHE:CZ	2.98	0.51
1:A:161:PHE:O	1:A:292:TYR:HB2	2.09	0.51
1:D:120:TYR:HA	1:D:136:ASN:O	2.10	0.51
1:D:132:LEU:HD21	1:D:320:LEU:HD12	1.92	0.51
1:B:264:PRO:O	1:B:268:VAL:HG22	2.09	0.51
1:B:130:ASN:O	1:B:132:LEU:CD1	2.58	0.51
1:D:267:LEU:HD12	1:D:267:LEU:N	2.25	0.51
1:B:246:ASP:CB	1:B:264:PRO:HB3	2.41	0.51
1:D:204:ARG:HD3	1:D:311:CYS:CA	2.40	0.51
1:C:237:ILE:O	1:C:241:MET:HB2	2.10	0.51
1:D:280:ASN:CG	1:D:281:GLY:H	2.14	0.51
1:A:252:ILE:HB	1:A:258:ILE:O	2.11	0.50
1:D:192:THR:CG2	1:D:315:HIS:NE2	2.75	0.50
1:B:88:LEU:N	1:B:88:LEU:HD12	2.26	0.50
1:A:124:HIS:NE2	1:A:172:PHE:CE1	2.76	0.50
1:B:265:GLU:O	1:B:268:VAL:HG23	2.12	0.50
1:A:266:THR:HG23	1:A:267:LEU:N	2.27	0.50
1:B:159:GLN:HG3	1:B:163:LEU:HD12	1.93	0.50
1:A:120:TYR:HA	1:A:136:ASN:O	2.12	0.50
1:B:266:THR:CG2	1:B:267:LEU:N	2.74	0.50
1:A:218:LEU:O	1:A:219:PRO:O	2.30	0.50
1:D:207:ILE:HD13	1:D:218:LEU:HD11	1.94	0.50
1:C:192:THR:CG2	1:C:315:HIS:NE2	2.74	0.49
1:A:315:HIS:ND1	1:A:317:PRO:HG3	2.27	0.49
1:B:311:CYS:C	1:B:313:THR:N	2.66	0.49
1:A:203:LEU:HD13	1:A:307:ILE:HG21	1.93	0.49
1:C:303:LEU:HD22	1:C:303:LEU:N	2.28	0.49
1:A:299:ALA:O	1:A:302:ASP:HB3	2.12	0.49
1:A:197:THR:O	1:A:201:GLY:N	2.46	0.49
1:A:54:ILE:CD1	1:D:54:ILE:HD11	2.41	0.49
1:D:303:LEU:N	1:D:303:LEU:HD22	2.27	0.49
1:B:134:ARG:CZ	1:B:136:ASN:HD21	2.26	0.49
1:C:214:ARG:NH1	1:C:321:PRO:CG	2.75	0.49
1:D:206:GLY:C	1:D:207:ILE:HD12	2.33	0.49
1:B:65:THR:N	1:B:66:PRO:CD	2.75	0.49
1:C:207:ILE:HD13	1:C:218:LEU:HD11	1.94	0.48
1:B:148:ARG:HH22	1:B:214:ARG:NH1	2.06	0.48
1:A:267:LEU:O	1:A:271:LEU:CD2	2.58	0.48
1:B:191:TRP:CD2	1:B:219:PRO:HG2	2.49	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:145:HIS:CE1	1:D:150:LEU:HD12	2.48	0.48
1:D:191:TRP:CE2	1:D:219:PRO:HB2	2.48	0.48
1:A:52:ARG:CZ	1:D:57:ASP:HA	2.44	0.48
1:D:130:ASN:O	1:D:132:LEU:HD13	2.13	0.48
1:B:246:ASP:HB2	1:B:264:PRO:HB3	1.95	0.48
1:C:267:LEU:N	1:C:267:LEU:HD12	2.29	0.48
1:B:148:ARG:HH12	1:B:214:ARG:NH2	2.06	0.48
1:C:262:GLU:HG3	1:C:282:GLN:CG	2.42	0.48
1:C:148:ARG:HH12	1:C:321:PRO:HA	1.74	0.48
1:B:82:ILE:HG22	1:B:83:SER:N	2.28	0.48
1:A:218:LEU:HD23	1:A:218:LEU:N	2.29	0.48
1:B:65:THR:N	1:B:66:PRO:HD2	2.29	0.48
1:D:237:ILE:O	1:D:241:MET:HB2	2.13	0.47
1:D:204:ARG:HD3	1:D:311:CYS:HA	1.96	0.47
1:B:120:TYR:HA	1:B:136:ASN:O	2.14	0.47
1:D:65:THR:N	1:D:66:PRO:CD	2.78	0.47
1:A:245:GLN:HA	1:A:301:GLY:HA2	1.97	0.47
1:D:237:ILE:HA	1:D:240:ILE:HG21	1.94	0.47
1:B:231:LEU:CG	1:B:232:THR:H	2.19	0.47
1:D:203:LEU:CB	1:D:309:GLN:HA	2.44	0.47
1:D:124:HIS:HD2	1:D:132:LEU:O	1.98	0.47
1:A:313:THR:HG21	1:C:255:THR:HG23	1.97	0.47
1:A:214:ARG:CD	1:A:314:CYS:HB2	2.45	0.47
1:A:296:ASP:OD1	1:A:297:PRO:CD	2.55	0.47
1:B:265:GLU:O	1:B:268:VAL:HG22	2.16	0.47
1:C:75:LEU:HD12	1:C:98:LEU:HD21	1.96	0.47
1:A:311:CYS:O	1:A:312:ASP:C	2.53	0.46
1:B:192:THR:O	1:B:193:ASP:CB	2.60	0.46
1:A:134:ARG:CZ	1:A:136:ASN:HD21	2.28	0.46
1:B:172:PHE:HE1	1:B:174:PHE:CE2	2.34	0.46
1:B:305:MET:HG2	1:B:306:VAL:N	2.29	0.46
1:C:213:LEU:HD11	1:C:293:ILE:HD11	1.97	0.46
1:B:131:PRO:C	1:B:132:LEU:HD12	2.36	0.46
1:A:49:ASN:HA	1:B:49:ASN:HA	1.96	0.46
1:D:157:PHE:CE1	1:D:319:SER:HB3	2.50	0.46
1:A:316:SER:N	1:A:317:PRO:CD	2.76	0.46
1:D:214:ARG:NH1	1:D:321:PRO:CG	2.79	0.46
1:C:130:ASN:O	1:C:132:LEU:HD13	2.16	0.46
1:B:140:PRO:HA	1:D:60:ASP:OD1	2.15	0.46
1:B:246:ASP:HB2	1:B:264:PRO:CB	2.45	0.46
1:A:142:ILE:N	1:A:142:ILE:HD12	2.31	0.46
1:A:65:THR:N	1:A:66:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:ASP:OD1	1:A:57:ASP:N	2.38	0.46
1:C:172:PHE:HE1	1:C:174:PHE:CE2	2.34	0.46
1:C:206:GLY:C	1:C:207:ILE:HD12	2.37	0.46
1:B:88:LEU:N	1:B:88:LEU:CD1	2.79	0.45
1:A:89:MET:HB2	1:A:92:ILE:HD12	1.92	0.45
1:C:120:TYR:HA	1:C:136:ASN:O	2.17	0.45
1:B:266:THR:O	1:B:269:HIS:HB3	2.16	0.45
1:A:216:ILE:HG22	1:A:285:ILE:HG21	1.97	0.45
1:B:192:THR:HA	1:B:219:PRO:HG3	1.98	0.45
1:C:307:ILE:O	1:C:307:ILE:HG22	2.14	0.45
1:A:134:ARG:NH2	1:A:136:ASN:HD21	2.15	0.45
1:A:268:VAL:O	1:A:269:HIS:C	2.54	0.45
1:B:190:THR:HG23	1:B:286:PRO:CG	2.46	0.45
1:A:209:PHE:HZ	1:A:289:LEU:HD21	1.80	0.45
1:D:148:ARG:HH12	1:D:321:PRO:HA	1.79	0.45
1:B:269:HIS:C	1:B:269:HIS:CD2	2.88	0.45
1:B:288:LEU:CD1	1:B:288:LEU:N	2.80	0.45
1:B:231:LEU:CD2	1:B:232:THR:N	2.43	0.45
1:B:131:PRO:O	1:B:132:LEU:HD12	2.17	0.45
1:D:172:PHE:HE2	1:D:174:PHE:CZ	2.34	0.44
1:B:130:ASN:O	1:B:132:LEU:HD13	2.17	0.44
1:B:312:ASP:O	1:B:312:ASP:OD1	2.36	0.44
1:A:130:ASN:O	1:A:132:LEU:HD13	2.17	0.44
1:D:134:ARG:NH2	1:D:136:ASN:HD21	2.16	0.44
1:C:191:TRP:CE2	1:C:219:PRO:HB2	2.51	0.44
1:C:214:ARG:NH1	1:C:321:PRO:HG3	2.32	0.44
1:D:192:THR:CG2	1:D:315:HIS:CE1	3.00	0.44
1:C:159:GLN:HG3	1:C:163:LEU:HD12	2.00	0.44
1:B:238:GLN:O	1:B:242:THR:HG23	2.17	0.44
1:D:131:PRO:HB2	1:D:159:GLN:OE1	2.17	0.44
1:D:184:GLN:HA	1:D:185:PRO:HD3	1.90	0.44
1:A:130:ASN:O	1:A:132:LEU:CD1	2.66	0.44
1:D:124:HIS:CE1	1:D:172:PHE:HE1	2.21	0.44
1:D:124:HIS:ND1	1:D:172:PHE:CD1	2.86	0.44
1:B:134:ARG:NH2	1:B:136:ASN:HD21	2.15	0.44
1:A:248:LYS:HB3	1:A:262:GLU:HG2	1.99	0.44
1:D:75:LEU:HD12	1:D:98:LEU:HD21	1.99	0.44
1:D:130:ASN:O	1:D:132:LEU:CD1	2.66	0.44
1:B:246:ASP:HB2	1:B:264:PRO:HG3	2.00	0.44
1:B:210:HIS:O	1:B:213:LEU:O	2.36	0.44
1:B:266:THR:CG2	1:B:267:LEU:H	2.30	0.43
1:D:267:LEU:CD1	1:D:267:LEU:H	2.31	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:311:CYS:O	1:A:313:THR:N	2.51	0.43
1:D:267:LEU:H	1:D:267:LEU:HD12	1.84	0.43
1:C:142:ILE:CG2	1:C:145:HIS:HB2	2.47	0.43
1:A:315:HIS:CE1	1:A:317:PRO:HD2	2.45	0.43
1:D:210:HIS:ND1	1:D:212:LYS:N	2.62	0.43
1:D:237:ILE:CA	1:D:240:ILE:CG2	2.94	0.43
1:C:65:THR:N	1:C:66:PRO:CD	2.81	0.43
1:B:203:LEU:C	1:B:203:LEU:HD12	2.39	0.43
1:C:247:PHE:CE2	1:C:263:VAL:HG12	2.54	0.43
1:D:131:PRO:C	1:D:132:LEU:HD12	2.38	0.43
1:A:122:ILE:HG22	1:A:174:PHE:CD2	2.54	0.43
1:D:142:ILE:HD12	1:D:142:ILE:N	2.33	0.43
1:C:124:HIS:CE1	1:C:172:PHE:CD2	3.05	0.43
1:A:54:ILE:HD11	1:D:54:ILE:CD1	2.46	0.43
1:A:200:ASN:ND2	1:C:252:ILE:HG12	2.33	0.43
1:A:156:ALA:HB2	1:A:315:HIS:HE1	1.81	0.43
1:D:124:HIS:ND1	1:D:172:PHE:CZ	2.87	0.43
1:C:290:PRO:HD3	1:C:318:ALA:HB2	2.01	0.43
1:B:265:GLU:C	1:B:268:VAL:HG22	2.38	0.42
1:B:204:ARG:HH11	1:B:217:LEU:HD13	1.83	0.42
1:A:164:PRO:HA	1:A:165:PRO:HD3	1.91	0.42
1:C:210:HIS:ND1	1:C:212:LYS:N	2.52	0.42
1:A:131:PRO:O	1:A:132:LEU:HD12	2.18	0.42
1:D:164:PRO:HA	1:D:165:PRO:HD3	1.89	0.42
1:B:74:ILE:HD13	1:B:95:TRP:CZ2	2.54	0.42
1:D:159:GLN:HG3	1:D:163:LEU:HD12	2.01	0.42
1:A:267:LEU:CD1	1:A:271:LEU:HD21	2.49	0.42
1:C:282:GLN:O	1:C:284:ILE:HG13	2.20	0.42
1:B:124:HIS:CG	1:B:172:PHE:CE2	3.08	0.42
1:D:103:GLN:HA	1:D:106:TYR:O	2.20	0.42
1:D:94:ILE:CG2	1:D:96:LEU:HD21	2.49	0.42
1:C:131:PRO:C	1:C:132:LEU:HD12	2.40	0.41
1:C:192:THR:CG2	1:C:315:HIS:CE1	3.03	0.41
1:D:280:ASN:CG	1:D:281:GLY:N	2.72	0.41
1:A:214:ARG:HA	1:A:215:PRO:HD3	1.92	0.41
1:D:288:LEU:N	1:D:288:LEU:HD12	2.35	0.41
1:B:244:LEU:O	1:B:244:LEU:HD12	2.19	0.41
1:D:124:HIS:NE2	1:D:172:PHE:CE1	2.84	0.41
1:A:243:SER:O	1:A:246:ASP:N	2.34	0.41
1:A:267:LEU:HD11	1:A:271:LEU:HD21	2.02	0.41
1:B:233:SER:HB3	1:B:235:GLU:OE2	2.20	0.41
1:C:285:ILE:HA	1:C:286:PRO:HD2	1.91	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:LEU:HD12	1:A:203:LEU:C	2.41	0.41
1:A:191:TRP:CZ3	1:A:263:VAL:HG21	2.56	0.41
1:A:191:TRP:HZ3	1:A:263:VAL:HG21	1.86	0.41
1:A:218:LEU:CD2	1:A:218:LEU:N	2.83	0.41
1:C:103:GLN:HA	1:C:106:TYR:O	2.20	0.41
1:D:320:LEU:HA	1:D:321:PRO:HD3	1.87	0.41
1:C:142:ILE:HD12	1:C:142:ILE:N	2.35	0.41
1:B:293:ILE:HG23	1:B:293:ILE:O	2.20	0.41
1:B:142:ILE:CG2	1:B:145:HIS:HB2	2.46	0.41
1:A:244:LEU:HA	1:A:247:PHE:CD1	2.56	0.41
1:D:232:THR:O	1:D:233:SER:C	2.58	0.41
1:C:134:ARG:HB3	1:C:134:ARG:HE	1.63	0.41
1:C:122:ILE:HG22	1:C:174:PHE:CD2	2.55	0.41
1:C:203:LEU:C	1:C:203:LEU:HD12	2.40	0.41
1:D:204:ARG:NH1	1:D:311:CYS:O	2.53	0.41
1:A:267:LEU:CD1	1:A:271:LEU:CD2	2.99	0.41
1:C:65:THR:N	1:C:66:PRO:HD2	2.36	0.41
1:B:309:GLN:HG3	1:D:251:PRO:HG3	2.03	0.41
1:B:116:MET:HE2	1:C:116:MET:CE	2.51	0.41
1:A:216:ILE:CG2	1:A:285:ILE:HG21	2.51	0.41
1:A:73:PHE:C	1:A:74:ILE:HG13	2.41	0.41
1:D:52:ARG:HD3	1:D:118:ALA:O	2.21	0.41
1:B:73:PHE:C	1:B:74:ILE:HG13	2.41	0.40
1:D:290:PRO:HD3	1:D:318:ALA:HB2	2.04	0.40
1:B:116:MET:CE	1:C:116:MET:CE	2.99	0.40
1:B:237:ILE:N	1:B:237:ILE:HD12	2.36	0.40
1:B:269:HIS:O	1:B:269:HIS:HD2	2.04	0.40
1:B:142:ILE:HD12	1:B:142:ILE:N	2.37	0.40
1:B:52:ARG:CZ	1:C:57:ASP:HA	2.51	0.40
1:C:267:LEU:H	1:C:267:LEU:HD12	1.87	0.40
1:D:94:ILE:HG22	1:D:96:LEU:HD21	2.02	0.40
1:C:158:LEU:HB2	1:C:161:PHE:CD2	2.56	0.40
1:B:231:LEU:HD23	1:B:232:THR:OG1	2.21	0.40
1:B:190:THR:HG23	1:B:286:PRO:HG3	2.03	0.40
1:B:59:ILE:HG21	1:C:117:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/297 (88%)	240 (92%)	18 (7%)	2 (1%)	27	74
1	B	241/297 (81%)	224 (93%)	16 (7%)	1 (0%)	43	84
1	C	225/297 (76%)	213 (95%)	11 (5%)	1 (0%)	43	84
1	D	223/297 (75%)	212 (95%)	11 (5%)	0	100	100
All	All	949/1188 (80%)	889 (94%)	56 (6%)	4 (0%)	43	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	PRO
1	A	269	HIS
1	B	312	ASP
1	C	85	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/259 (90%)	231 (99%)	2 (1%)	87	97
1	B	219/259 (85%)	218 (100%)	1 (0%)	94	98
1	C	208/259 (80%)	208 (100%)	0	100	100
1	D	208/259 (80%)	207 (100%)	1 (0%)	94	98
All	All	868/1036 (84%)	864 (100%)	4 (0%)	94	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	LEU
1	A	221	LYS
1	B	278	SER
1	D	269	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	136	ASN
1	A	315	HIS
1	B	124	HIS
1	B	136	ASN
1	B	269	HIS
1	B	309	GLN
1	C	124	HIS
1	C	136	ASN
1	C	245	GLN
1	D	124	HIS
1	D	136	ASN
1	D	245	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	266/297 (89%)	-0.33	0 100 100	24, 64, 93, 109	0
1	B	249/297 (83%)	-0.32	0 100 100	38, 66, 99, 109	0
1	C	237/297 (79%)	-0.29	0 100 100	38, 64, 103, 118	0
1	D	235/297 (79%)	-0.30	0 100 100	38, 64, 103, 119	0
All	All	987/1188 (83%)	-0.31	0 100 100	24, 65, 100, 119	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.