wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:58 PM BST

PDB ID	:	4UOM
EMDB ID:	:	EMD-2645
Title	:	Electron Cryo-microscopy of Venezuelan Equine Encephalitis Virus TC- 83 in complex with neutralizing antibody Fab F5
Authors	:	Porta, J.; Jose, J.; Roehrig, J.T.; Blair, C.D.; Kuhn, R.J.; Rossmann, M.G.
Deposited on	:	2014-06-05
Resolution	:	17.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

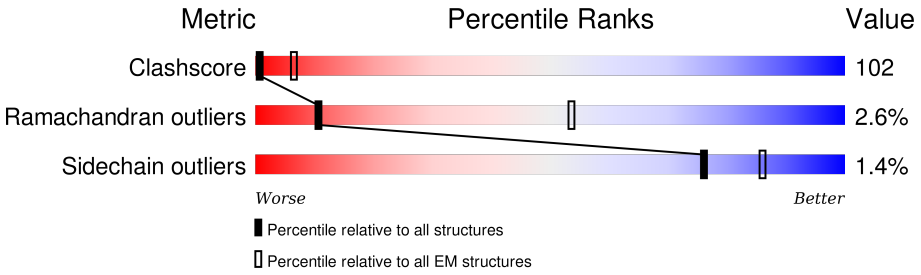
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 <=5%

Mol	Chain	Length	Quality of chain
1	H	217	54% 42% .
2	L	205	58% 29% 7% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3206 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	217	1645	1045	265	328	7	0	0

- Molecule 2 is a protein called FAB FRAGMENT LIGHT CHAIN.

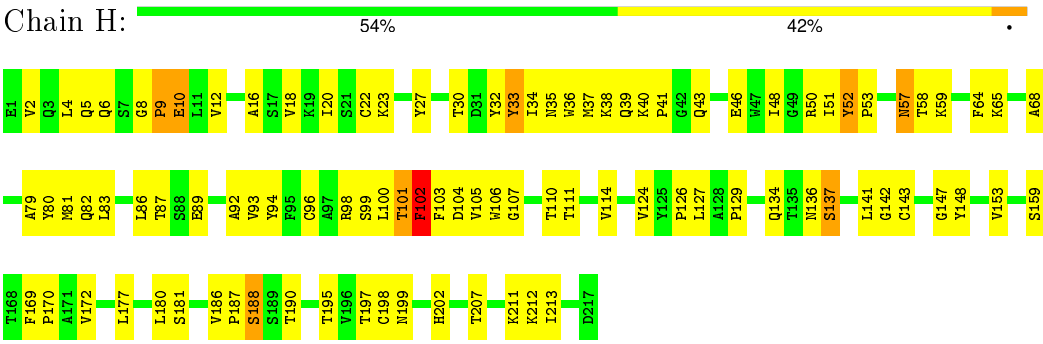
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	205	1561	969	262	325	5	0	0

3 Residue-property plots (i)

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. 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. 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.

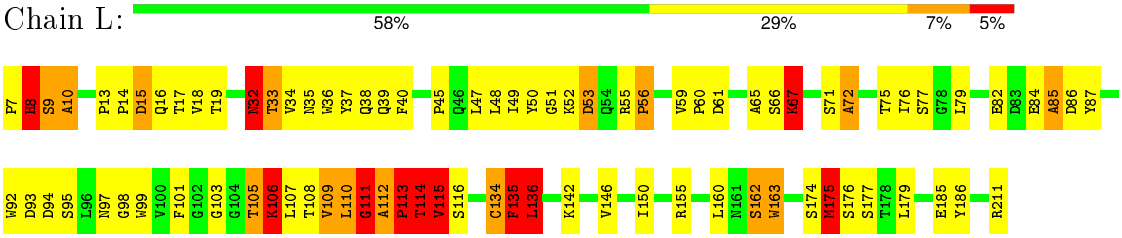
- Molecule 1: FAB FRAGMENT HEAVY CHAIN

Chain H:



- Molecule 2: FAB FRAGMENT LIGHT CHAIN

Chain L:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH IMAGE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	24	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	H	0.77	1/1689 (0.1%)	1.08	9/2309 (0.4%)
2	L	4.12	53/1600 (3.3%)	2.24	78/2177 (3.6%)
All	All	2.93	54/3289 (1.6%)	1.75	87/4486 (1.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	2
2	L	3	8
All	All	3	10

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	111	GLY	CA-C	76.78	2.74	1.51
2	L	163	TRP	CD2-CE2	72.59	2.28	1.41
2	L	111	GLY	N-CA	-39.51	0.86	1.46
2	L	113	PRO	CG-CD	-31.23	0.47	1.50
2	L	112	ALA	CA-CB	-29.16	0.91	1.52
2	L	175	MET	CG-SD	29.15	2.56	1.81
2	L	113	PRO	N-CD	28.77	1.88	1.47
2	L	134	CYS	C-N	28.56	1.99	1.34
2	L	111	GLY	C-O	-25.39	0.83	1.23
2	L	114	THR	N-CA	-24.47	0.97	1.46
2	L	114	THR	CB-CG2	-22.12	0.79	1.52
2	L	163	TRP	NE1-CE2	21.98	1.66	1.37
2	L	114	THR	CA-CB	21.07	2.08	1.53
2	L	135	PHE	N-CA	20.38	1.87	1.46
2	L	175	MET	CB-CG	-19.80	0.88	1.51
2	L	163	TRP	CG-CD1	19.57	1.64	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	112	ALA	N-CA	-19.18	1.07	1.46
2	L	114	THR	CA-C	18.40	2.00	1.52
2	L	163	TRP	CG-CD2	18.39	1.75	1.43
2	L	106	LYS	N-CA	-17.86	1.10	1.46
2	L	112	ALA	C-N	16.75	1.66	1.34
2	L	114	THR	CB-OG1	16.40	1.76	1.43
2	L	106	LYS	CB-CG	-16.38	1.08	1.52
2	L	112	ALA	C-O	-15.49	0.94	1.23
2	L	114	THR	C-O	-15.40	0.94	1.23
2	L	134	CYS	CA-CB	-15.39	1.20	1.53
2	L	113	PRO	N-CA	-15.20	1.21	1.47
2	L	163	TRP	CD1-NE1	14.83	1.63	1.38
1	H	57	ASN	C-O	-14.31	0.96	1.23
2	L	163	TRP	CD2-CE3	-13.28	1.20	1.40
2	L	106	LYS	CE-NZ	-13.08	1.16	1.49
2	L	106	LYS	C-O	-13.03	0.98	1.23
2	L	135	PHE	CA-CB	-12.28	1.26	1.53
2	L	134	CYS	C-O	11.37	1.45	1.23
2	L	112	ALA	CA-C	11.03	1.81	1.52
2	L	106	LYS	CG-CD	-10.93	1.15	1.52
2	L	56	PRO	N-CD	-9.97	1.33	1.47
2	L	175	MET	CA-CB	-9.80	1.32	1.53
2	L	136	LEU	CG-CD1	-9.73	1.15	1.51
2	L	106	LYS	CA-C	7.68	1.73	1.52
2	L	67	LYS	CG-CD	-7.51	1.26	1.52
2	L	135	PHE	C-N	-6.89	1.18	1.34
2	L	163	TRP	CE2-CZ2	-6.85	1.28	1.39
2	L	110	LEU	C-O	-6.73	1.10	1.23
2	L	163	TRP	CB-CG	-6.24	1.39	1.50
2	L	175	MET	SD-CE	6.21	2.12	1.77
2	L	33	THR	CB-CG2	-5.92	1.32	1.52
2	L	9	SER	CA-C	-5.88	1.37	1.52
2	L	110	LEU	C-N	-5.60	1.23	1.33
2	L	134	CYS	CA-C	5.53	1.67	1.52
2	L	113	PRO	C-N	-5.48	1.21	1.34
2	L	32	ASN	CB-CG	-5.19	1.39	1.51
2	L	8	HIS	C-O	-5.16	1.13	1.23
2	L	135	PHE	CA-C	-5.14	1.39	1.52

All (87) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	113	PRO	N-CD-CG	27.36	144.24	103.20
2	L	163	TRP	NE1-CE2-CZ2	25.77	158.75	130.40
2	L	135	PHE	CA-C-N	20.80	162.97	117.20
2	L	135	PHE	CA-C-O	-20.63	76.78	120.10
2	L	113	PRO	N-CA-CB	-19.55	79.83	103.30
2	L	113	PRO	CA-N-CD	-16.75	88.05	111.50
2	L	175	MET	CG-SD-CE	16.69	126.90	100.20
2	L	112	ALA	N-CA-CB	16.17	132.73	110.10
2	L	163	TRP	CD2-CE2-CZ2	-16.13	102.94	122.30
2	L	135	PHE	O-C-N	-16.11	96.92	122.70
2	L	112	ALA	CA-C-O	-15.58	87.38	120.10
2	L	163	TRP	NE1-CE2-CD2	-15.03	92.27	107.30
2	L	175	MET	CB-CG-SD	14.91	157.13	112.40
2	L	9	SER	N-CA-C	14.87	151.13	111.00
2	L	10	ALA	N-CA-CB	13.82	129.45	110.10
2	L	106	LYS	O-C-N	-13.70	100.78	122.70
2	L	163	TRP	CD1-NE1-CE2	13.22	120.89	109.00
2	L	134	CYS	N-CA-CB	12.56	133.22	110.60
2	L	111	GLY	N-CA-C	12.14	143.44	113.10
2	L	67	LYS	CG-CD-CE	12.11	148.21	111.90
2	L	111	GLY	CA-C-O	11.82	141.89	120.60
2	L	135	PHE	CB-CA-C	11.69	133.78	110.40
2	L	134	CYS	CB-CA-C	-11.47	87.47	110.40
2	L	8	HIS	CB-CA-C	-10.81	88.79	110.40
1	H	102	PHE	CB-CG-CD1	-10.55	113.42	120.80
1	H	101	THR	CA-CB-CG2	10.51	127.12	112.40
2	L	136	LEU	CB-CG-CD1	9.77	127.62	111.00
2	L	134	CYS	CA-C-O	-8.82	101.58	120.10
2	L	114	THR	C-N-CA	8.75	143.58	121.70
2	L	163	TRP	CA-CB-CG	8.58	130.01	113.70
2	L	112	ALA	CB-CA-C	-8.11	97.94	110.10
2	L	175	MET	N-CA-CB	-8.02	96.17	110.60
2	L	111	GLY	O-C-N	-7.73	110.33	122.70
2	L	135	PHE	CA-CB-CG	7.59	132.12	113.90
2	L	114	THR	O-C-N	-7.51	110.68	122.70
2	L	163	TRP	CZ3-CH2-CZ2	7.45	130.54	121.60
2	L	8	HIS	C-N-CA	7.40	140.20	121.70
2	L	106	LYS	CA-CB-CG	7.29	129.44	113.40
2	L	8	HIS	O-C-N	7.19	134.20	122.70
2	L	175	MET	CB-CA-C	7.16	124.73	110.40
2	L	72	ALA	N-CA-CB	-7.16	100.08	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	135	PHE	N-CA-CB	7.09	123.37	110.60
2	L	8	HIS	CA-C-O	-7.09	105.22	120.10
2	L	113	PRO	CB-CG-CD	-6.94	79.42	106.50
2	L	10	ALA	CB-CA-C	-6.81	99.88	110.10
2	L	106	LYS	N-CA-CB	6.77	122.79	110.60
2	L	56	PRO	N-CD-CG	6.75	113.32	103.20
2	L	32	ASN	CB-CG-OD1	-6.73	108.14	121.60
2	L	112	ALA	CA-C-N	6.67	135.78	117.10
2	L	135	PHE	C-N-CA	6.56	138.11	121.70
2	L	9	SER	CA-C-O	-6.47	106.52	120.10
2	L	115	VAL	CG1-CB-CG2	-6.43	100.60	110.90
2	L	114	THR	CA-C-N	6.43	131.34	117.20
1	H	58	THR	CA-CB-CG2	6.41	121.37	112.40
2	L	115	VAL	N-CA-CB	-6.38	97.47	111.50
2	L	33	THR	OG1-CB-CG2	6.25	124.37	110.00
2	L	135	PHE	CB-CG-CD1	6.25	125.17	120.80
2	L	115	VAL	N-CA-C	6.22	127.79	111.00
2	L	67	LYS	CD-CE-NZ	6.11	125.76	111.70
2	L	163	TRP	CE2-CD2-CG	-6.09	102.43	107.30
2	L	32	ASN	CB-CA-C	6.08	122.56	110.40
2	L	175	MET	O-C-N	-6.07	112.98	122.70
2	L	10	ALA	N-CA-C	6.06	127.37	111.00
2	L	9	SER	CB-CA-C	-5.92	98.86	110.10
1	H	102	PHE	CD1-CG-CD2	5.79	125.83	118.30
2	L	110	LEU	C-N-CA	-5.77	110.18	122.30
2	L	113	PRO	N-CA-C	5.77	127.09	112.10
2	L	9	SER	CA-CB-OG	-5.75	95.68	111.20
2	L	112	ALA	N-CA-C	5.66	126.27	111.00
2	L	115	VAL	CA-C-N	-5.65	104.78	117.20
2	L	135	PHE	CB-CG-CD2	-5.63	116.86	120.80
2	L	112	ALA	C-N-CA	5.61	145.57	122.00
1	H	188	SER	CB-CA-C	-5.60	99.45	110.10
2	L	106	LYS	CA-C-O	5.54	131.73	120.10
2	L	67	LYS	CB-CG-CD	5.43	125.73	111.60
1	H	57	ASN	C-N-CA	-5.41	108.17	121.70
1	H	52	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	H	57	ASN	N-CA-C	5.40	125.57	111.00
1	H	110	THR	CA-CB-CG2	5.32	119.85	112.40
2	L	162	SER	CB-CA-C	-5.30	100.02	110.10
2	L	110	LEU	CA-C-O	5.30	131.23	120.10
2	L	163	TRP	CG-CD2-CE3	5.27	138.64	133.90
2	L	105	THR	O-C-N	5.20	131.02	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	175	MET	CA-CB-CG	5.19	122.12	113.30
2	L	32	ASN	CA-CB-CG	5.16	124.75	113.40
2	L	113	PRO	CB-CA-C	5.11	124.77	112.00
2	L	53	ASP	CB-CG-OD1	5.02	122.82	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	L	9	SER	CA
2	L	112	ALA	CA
2	L	135	PHE	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	33	TYR	Sidechain
1	H	9	PRO	Mainchain
2	L	106	LYS	Mainchain
2	L	111	GLY	Peptide
2	L	113	PRO	Mainchain
2	L	114	THR	Peptide
2	L	115	VAL	Mainchain
2	L	135	PHE	Mainchain
2	L	175	MET	Mainchain
2	L	8	HIS	Mainchain

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	H	1645	0	1608	164	0
2	L	1561	0	1463	533	0
All	All	3206	0	3071	641	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 102.

All (641) 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)
2:L:163:TRP:CD2	2:L:163:TRP:CG	1.74	1.59
2:L:111:GLY:C	2:L:163:TRP:CD2	1.80	1.54
2:L:111:GLY:CA	2:L:163:TRP:CE2	1.91	1.53
2:L:111:GLY:C	2:L:163:TRP:CE2	1.78	1.53
1:H:37:MET:CE	2:L:101:PHE:HZ	1.25	1.50
2:L:111:GLY:CA	2:L:163:TRP:CD2	1.96	1.48
2:L:112:ALA:C	2:L:112:ALA:CA	1.81	1.47
2:L:175:MET:CG	2:L:175:MET:CA	1.93	1.44
2:L:112:ALA:N	2:L:112:ALA:CB	1.82	1.38
2:L:114:THR:C	2:L:136:LEU:HD12	1.42	1.37
2:L:175:MET:SD	2:L:175:MET:CE	2.12	1.37
2:L:135:PHE:N	2:L:135:PHE:CA	1.87	1.37
1:H:37:MET:CE	2:L:101:PHE:CZ	2.08	1.33
2:L:114:THR:OG1	2:L:114:THR:CB	1.76	1.31
2:L:114:THR:CA	2:L:114:THR:CB	2.08	1.29
2:L:114:THR:C	2:L:135:PHE:O	1.68	1.29
2:L:114:THR:C	2:L:114:THR:CA	2.00	1.28
2:L:114:THR:HB	2:L:135:PHE:CG	1.66	1.28
2:L:55:ARG:NH1	2:L:61:ASP:HA	1.50	1.26
2:L:32:ASN:HB2	2:L:33:THR:CB	1.66	1.24
1:H:37:MET:HE1	2:L:101:PHE:CZ	1.70	1.23
2:L:111:GLY:C	2:L:163:TRP:CG	2.10	1.23
2:L:163:TRP:CD2	2:L:163:TRP:CE2	2.28	1.21
2:L:113:PRO:HD3	2:L:175:MET:SD	1.82	1.19
1:H:50:ARG:NH2	2:L:99:TRP:CE3	2.09	1.19
2:L:111:GLY:HA2	2:L:163:TRP:CE2	1.68	1.18
2:L:7:PRO:O	2:L:106:LYS:HB3	1.41	1.16
2:L:111:GLY:C	2:L:163:TRP:CD1	2.19	1.16
2:L:92:TRP:HB3	2:L:95:SER:HB2	1.24	1.15
2:L:112:ALA:C	2:L:112:ALA:CB	2.14	1.15
2:L:134:CYS:C	2:L:135:PHE:N	1.99	1.14
2:L:113:PRO:HB3	2:L:175:MET:CE	1.77	1.14
2:L:111:GLY:HA2	2:L:163:TRP:CZ2	1.83	1.14
2:L:115:VAL:HG23	2:L:136:LEU:CG	1.76	1.14
2:L:111:GLY:O	2:L:175:MET:HG3	1.47	1.13
2:L:112:ALA:N	2:L:163:TRP:CE2	2.15	1.13
2:L:9:SER:N	2:L:106:LYS:HB2	1.63	1.12
2:L:113:PRO:CB	2:L:136:LEU:HD13	1.79	1.12
2:L:67:LYS:HB2	2:L:71:SER:O	1.49	1.12
2:L:111:GLY:O	2:L:112:ALA:N	1.83	1.11
2:L:67:LYS:CB	2:L:72:ALA:HA	1.79	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:111:GLY:C	2:L:163:TRP:NE1	2.03	1.10
1:H:172:VAL:HG11	2:L:160:LEU:HD22	1.20	1.10
2:L:109:VAL:HG23	2:L:142:LYS:HE2	1.32	1.10
2:L:93:ASP:HB2	2:L:99:TRP:CE3	1.87	1.10
2:L:48:LEU:O	2:L:56:PRO:HD2	1.49	1.09
1:H:37:MET:HE3	2:L:101:PHE:HZ	1.14	1.09
2:L:114:THR:C	2:L:135:PHE:N	2.06	1.09
2:L:112:ALA:N	2:L:163:TRP:CD2	2.21	1.08
1:H:38:LYS:HB2	1:H:48:ILE:HD11	1.23	1.08
2:L:86:ASP:CA	2:L:105:THR:HG21	1.82	1.08
1:H:172:VAL:CG1	2:L:160:LEU:HD22	1.84	1.08
2:L:112:ALA:C	2:L:175:MET:SD	2.32	1.08
2:L:113:PRO:HB3	2:L:175:MET:HE2	1.11	1.07
2:L:92:TRP:HE1	2:L:94:ASP:HB2	1.10	1.07
2:L:115:VAL:CG2	2:L:136:LEU:HG	1.85	1.06
2:L:86:ASP:HA	2:L:105:THR:HG21	1.09	1.06
2:L:112:ALA:HA	2:L:112:ALA:CB	1.59	1.06
2:L:112:ALA:CA	2:L:112:ALA:O	2.00	1.05
2:L:34:VAL:HG11	2:L:67:LYS:HE3	1.35	1.05
2:L:135:PHE:N	2:L:135:PHE:O	1.88	1.05
2:L:112:ALA:HB2	2:L:112:ALA:CA	1.53	1.05
2:L:114:THR:CB	2:L:135:PHE:N	2.20	1.04
2:L:112:ALA:HB1	2:L:112:ALA:C	1.78	1.04
2:L:32:ASN:HB2	2:L:33:THR:HB	1.34	1.04
2:L:114:THR:HG1	2:L:135:PHE:N	1.55	1.04
2:L:175:MET:CA	2:L:175:MET:HG2	1.72	1.04
2:L:49:ILE:HD13	2:L:65:ALA:HB2	1.37	1.04
2:L:114:THR:CA	2:L:134:CYS:C	2.26	1.04
2:L:92:TRP:NE1	2:L:94:ASP:HB2	1.73	1.04
2:L:8:HIS:C	2:L:106:LYS:HB2	1.78	1.03
2:L:111:GLY:CA	2:L:163:TRP:NE1	2.22	1.03
2:L:113:PRO:CD	2:L:175:MET:SD	2.46	1.03
2:L:114:THR:HB	2:L:135:PHE:CB	1.87	1.03
2:L:111:GLY:O	2:L:111:GLY:C	0.83	1.02
2:L:38:GLN:CD	2:L:48:LEU:HD21	1.78	1.02
1:H:37:MET:HE1	2:L:101:PHE:HZ	1.02	1.02
2:L:34:VAL:HG21	2:L:67:LYS:NZ	1.74	1.02
2:L:112:ALA:HB1	2:L:112:ALA:CA	1.53	1.01
2:L:112:ALA:N	2:L:175:MET:SD	2.33	1.01
2:L:114:THR:CA	2:L:135:PHE:N	2.22	1.01
1:H:6:GLN:HE22	1:H:107:GLY:HA3	1.22	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:112:ALA:C	2:L:175:MET:HG2	1.80	1.01
2:L:67:LYS:HB3	2:L:72:ALA:HA	1.39	1.00
2:L:112:ALA:HB3	2:L:112:ALA:CA	1.53	0.99
2:L:111:GLY:O	2:L:163:TRP:CD1	2.15	0.99
1:H:102:PHE:CE1	2:L:50:TYR:HB3	1.96	0.99
2:L:109:VAL:CG2	2:L:142:LYS:HE2	1.92	0.99
2:L:175:MET:CG	2:L:175:MET:HB3	1.48	0.99
2:L:111:GLY:N	2:L:163:TRP:CD2	2.31	0.99
2:L:175:MET:HB2	2:L:175:MET:CG	1.48	0.98
2:L:86:ASP:HA	2:L:105:THR:CG2	1.94	0.98
2:L:114:THR:HG23	2:L:134:CYS:O	1.64	0.98
2:L:114:THR:CG2	2:L:135:PHE:CD1	2.47	0.98
2:L:32:ASN:HB2	2:L:33:THR:CA	1.93	0.97
2:L:33:THR:HG21	2:L:95:SER:HB2	1.44	0.97
2:L:106:LYS:C	2:L:107:LEU:HD12	1.84	0.97
2:L:114:THR:C	2:L:135:PHE:C	2.22	0.97
2:L:7:PRO:HD2	2:L:106:LYS:HE2	1.46	0.97
2:L:114:THR:O	2:L:134:CYS:SG	2.24	0.96
2:L:114:THR:HG22	2:L:114:THR:CB	1.44	0.96
2:L:110:LEU:O	2:L:163:TRP:CG	2.19	0.95
2:L:114:THR:CB	2:L:134:CYS:C	2.34	0.95
2:L:33:THR:OG1	2:L:92:TRP:HB2	1.67	0.95
2:L:113:PRO:HB2	2:L:136:LEU:HD13	1.44	0.94
2:L:115:VAL:N	2:L:135:PHE:C	2.20	0.94
1:H:170:PRO:HG2	2:L:162:SER:OG	1.67	0.94
1:H:102:PHE:CD1	2:L:50:TYR:HB3	2.03	0.94
2:L:175:MET:SD	2:L:175:MET:CG	2.57	0.94
2:L:114:THR:HG21	2:L:114:THR:CB	1.44	0.93
2:L:112:ALA:CA	2:L:175:MET:CG	2.46	0.93
2:L:114:THR:HG23	2:L:114:THR:CB	1.44	0.93
2:L:114:THR:HG22	2:L:135:PHE:CD1	2.04	0.93
2:L:114:THR:OG1	2:L:134:CYS:C	2.05	0.93
2:L:114:THR:C	2:L:136:LEU:CD1	2.37	0.93
2:L:113:PRO:N	2:L:175:MET:CG	2.32	0.93
2:L:114:THR:HB	2:L:135:PHE:CA	1.98	0.93
2:L:17:THR:HG22	2:L:77:SER:O	1.68	0.93
2:L:10:ALA:HB2	2:L:106:LYS:NZ	1.84	0.92
2:L:112:ALA:CA	2:L:175:MET:SD	2.57	0.92
2:L:113:PRO:CD	2:L:175:MET:CG	2.47	0.92
2:L:113:PRO:N	2:L:175:MET:HG2	1.83	0.92
2:L:114:THR:CB	2:L:135:PHE:CA	2.48	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:87:TYR:O	2:L:105:THR:HB	1.70	0.91
2:L:34:VAL:HG21	2:L:67:LYS:HZ2	1.29	0.91
2:L:112:ALA:CA	2:L:112:ALA:CB	0.91	0.91
2:L:175:MET:HG2	2:L:175:MET:CB	1.38	0.90
2:L:114:THR:HB	2:L:135:PHE:CD1	2.05	0.90
2:L:114:THR:OG1	2:L:135:PHE:N	2.04	0.90
2:L:112:ALA:C	2:L:175:MET:CG	2.39	0.89
2:L:7:PRO:CD	2:L:106:LYS:HE2	2.02	0.89
2:L:113:PRO:HB2	2:L:136:LEU:CD1	2.01	0.89
1:H:50:ARG:HG2	1:H:59:LYS:HB2	1.52	0.89
2:L:55:ARG:HH11	2:L:61:ASP:HA	1.18	0.89
2:L:175:MET:CB	2:L:175:MET:HG3	1.38	0.89
2:L:113:PRO:CA	2:L:136:LEU:HD13	2.01	0.89
1:H:35:ASN:HD22	1:H:103:PHE:HE1	1.21	0.88
2:L:106:LYS:O	2:L:107:LEU:HD12	1.71	0.88
2:L:112:ALA:HB3	2:L:162:SER:C	1.94	0.88
2:L:111:GLY:O	2:L:163:TRP:CG	2.26	0.88
2:L:33:THR:HG21	2:L:95:SER:CB	2.03	0.88
2:L:112:ALA:CB	2:L:162:SER:C	2.42	0.88
2:L:115:VAL:HG23	2:L:136:LEU:HG	0.91	0.88
2:L:114:THR:CA	2:L:114:THR:CG2	2.52	0.88
2:L:175:MET:CG	2:L:175:MET:CB	0.88	0.87
2:L:87:TYR:H	2:L:105:THR:CB	1.87	0.87
2:L:10:ALA:HB2	2:L:106:LYS:HZ1	1.38	0.87
2:L:112:ALA:HA	2:L:163:TRP:CE3	2.09	0.87
2:L:114:THR:OG1	2:L:114:THR:CG2	2.23	0.87
2:L:110:LEU:O	2:L:142:LYS:HE3	1.74	0.87
2:L:93:ASP:HB2	2:L:99:TRP:HE3	1.38	0.87
2:L:93:ASP:CA	2:L:99:TRP:HB3	2.05	0.86
2:L:10:ALA:CB	2:L:106:LYS:HZ2	1.87	0.86
2:L:110:LEU:C	2:L:142:LYS:HE3	1.96	0.86
2:L:114:THR:HB	2:L:114:THR:CG2	1.36	0.86
2:L:9:SER:CA	2:L:106:LYS:O	2.24	0.86
2:L:93:ASP:HA	2:L:99:TRP:HB3	1.58	0.85
2:L:49:ILE:CD1	2:L:65:ALA:HB2	2.06	0.85
2:L:85:ALA:O	2:L:107:LEU:HD22	1.77	0.85
2:L:18:VAL:HG12	2:L:76:ILE:HB	1.57	0.85
1:H:37:MET:HE3	2:L:101:PHE:CZ	1.95	0.84
2:L:10:ALA:CA	2:L:106:LYS:HZ2	1.90	0.84
2:L:55:ARG:NH1	2:L:61:ASP:CA	2.39	0.84
2:L:7:PRO:C	2:L:106:LYS:HB3	1.98	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:PRO:C	2:L:106:LYS:HD3	1.97	0.84
1:H:169:PHE:CE2	2:L:175:MET:C	2.52	0.83
2:L:112:ALA:CA	2:L:175:MET:HG3	2.08	0.83
2:L:113:PRO:C	2:L:136:LEU:HD13	1.99	0.83
2:L:113:PRO:HG2	2:L:136:LEU:CG	2.08	0.83
2:L:7:PRO:HG2	2:L:106:LYS:CE	2.08	0.83
2:L:10:ALA:CB	2:L:106:LYS:NZ	2.41	0.83
2:L:105:THR:HG23	2:L:105:THR:O	1.76	0.83
2:L:55:ARG:HH12	2:L:61:ASP:HA	1.44	0.83
2:L:67:LYS:HZ3	2:L:72:ALA:HB1	1.43	0.82
2:L:113:PRO:HD3	2:L:175:MET:CG	2.09	0.82
2:L:111:GLY:HA3	2:L:163:TRP:NE1	1.92	0.82
2:L:114:THR:CB	2:L:135:PHE:CG	2.59	0.82
2:L:52:LYS:HD2	2:L:67:LYS:O	1.79	0.82
2:L:93:ASP:CB	2:L:99:TRP:CE3	2.62	0.81
1:H:33:TYR:CD1	1:H:53:PRO:HD2	2.16	0.81
2:L:112:ALA:O	2:L:175:MET:HE3	1.81	0.81
2:L:113:PRO:CB	2:L:146:VAL:HG21	2.10	0.81
2:L:114:THR:CB	2:L:134:CYS:O	2.28	0.81
2:L:114:THR:OG1	2:L:134:CYS:CA	2.29	0.81
1:H:172:VAL:HG11	2:L:160:LEU:CD2	2.08	0.81
2:L:146:VAL:HG21	2:L:175:MET:HE2	1.62	0.80
2:L:49:ILE:HD13	2:L:65:ALA:CB	2.10	0.80
2:L:8:HIS:O	2:L:106:LYS:CA	2.29	0.80
2:L:111:GLY:CA	2:L:163:TRP:CZ2	2.47	0.80
2:L:39:GLN:O	2:L:85:ALA:HB1	1.81	0.80
2:L:110:LEU:O	2:L:142:LYS:CE	2.30	0.80
2:L:8:HIS:O	2:L:106:LYS:C	2.20	0.80
1:H:37:MET:HE1	2:L:101:PHE:CE1	2.17	0.80
2:L:7:PRO:HG2	2:L:106:LYS:HE2	1.62	0.80
1:H:170:PRO:CG	2:L:162:SER:OG	2.30	0.79
2:L:32:ASN:CB	2:L:33:THR:HB	2.12	0.79
1:H:6:GLN:NE2	1:H:107:GLY:HA3	1.97	0.79
2:L:112:ALA:N	2:L:163:TRP:CE3	2.50	0.79
1:H:101:THR:H	1:H:102:PHE:HB3	1.48	0.79
2:L:114:THR:CG2	2:L:114:THR:CB	0.79	0.79
2:L:7:PRO:HD2	2:L:106:LYS:CE	2.12	0.79
2:L:113:PRO:N	2:L:175:MET:SD	2.56	0.79
2:L:112:ALA:HB2	2:L:175:MET:HG3	1.65	0.79
2:L:67:LYS:HD2	2:L:72:ALA:CB	2.13	0.78
1:H:33:TYR:CE2	1:H:52:TYR:HB2	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:111:GLY:CA	2:L:163:TRP:CG	2.66	0.78
2:L:110:LEU:O	2:L:142:LYS:NZ	2.14	0.78
2:L:113:PRO:HD2	2:L:175:MET:HB3	1.65	0.78
2:L:113:PRO:HG2	2:L:136:LEU:HD22	1.64	0.78
2:L:110:LEU:N	2:L:142:LYS:HE3	1.99	0.78
2:L:8:HIS:O	2:L:106:LYS:HA	1.84	0.78
1:H:169:PHE:CD1	2:L:176:SER:HB2	2.19	0.77
2:L:112:ALA:N	2:L:163:TRP:CZ2	2.51	0.77
2:L:33:THR:HG23	2:L:33:THR:O	1.85	0.77
2:L:111:GLY:O	2:L:112:ALA:CA	2.32	0.76
2:L:7:PRO:CA	2:L:106:LYS:HD3	2.14	0.76
2:L:7:PRO:CG	2:L:106:LYS:HE2	2.15	0.76
1:H:37:MET:SD	2:L:101:PHE:CZ	2.79	0.76
2:L:113:PRO:HB3	2:L:146:VAL:HG21	1.68	0.76
2:L:38:GLN:NE2	2:L:48:LEU:HD21	2.00	0.76
2:L:113:PRO:CB	2:L:136:LEU:CD1	2.61	0.75
2:L:33:THR:HG21	2:L:92:TRP:HB3	1.68	0.75
2:L:34:VAL:CG2	2:L:67:LYS:NZ	2.48	0.75
2:L:114:THR:CG2	2:L:134:CYS:O	2.35	0.75
2:L:114:THR:CA	2:L:136:LEU:HD12	2.16	0.75
2:L:8:HIS:CA	2:L:106:LYS:HB2	2.16	0.75
2:L:87:TYR:N	2:L:105:THR:CB	2.50	0.75
2:L:112:ALA:O	2:L:175:MET:SD	2.44	0.75
2:L:111:GLY:C	2:L:175:MET:HG3	2.05	0.75
2:L:111:GLY:C	2:L:112:ALA:CB	2.54	0.75
1:H:159:SER:H	1:H:199:ASN:HD21	1.35	0.75
2:L:18:VAL:HG11	2:L:76:ILE:HD12	1.69	0.74
1:H:30:THR:HG22	1:H:74:THR:HB	1.68	0.74
2:L:163:TRP:CD2	2:L:163:TRP:CD1	2.75	0.74
2:L:113:PRO:CG	2:L:136:LEU:HD22	2.18	0.74
2:L:110:LEU:CA	2:L:142:LYS:HE3	2.17	0.74
2:L:114:THR:HG21	2:L:135:PHE:CD1	2.22	0.74
1:H:18:VAL:HG12	1:H:86:LEU:HD11	1.69	0.74
2:L:113:PRO:CG	2:L:175:MET:SD	2.67	0.74
2:L:8:HIS:C	2:L:106:LYS:CB	2.55	0.74
2:L:112:ALA:CB	2:L:162:SER:O	2.35	0.73
2:L:111:GLY:CA	2:L:163:TRP:CD1	2.71	0.73
2:L:38:GLN:OE1	2:L:48:LEU:HD11	1.88	0.73
1:H:167:HIS:CD2	2:L:174:SER:HG	2.07	0.73
2:L:114:THR:CB	2:L:135:PHE:O	2.34	0.73
2:L:40:PHE:HA	2:L:85:ALA:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:LEU:HD12	1:H:80:TYR:O	1.89	0.72
2:L:114:THR:O	2:L:136:LEU:HD12	1.82	0.72
2:L:112:ALA:O	2:L:175:MET:CE	2.37	0.72
1:H:6:GLN:HE21	1:H:96:CYS:H	1.37	0.72
2:L:105:THR:O	2:L:107:LEU:N	2.23	0.72
2:L:87:TYR:N	2:L:105:THR:HB	2.05	0.72
2:L:18:VAL:CG1	2:L:76:ILE:HB	2.19	0.72
2:L:114:THR:N	2:L:136:LEU:CD1	2.53	0.72
2:L:112:ALA:CB	2:L:175:MET:CG	2.68	0.72
2:L:9:SER:O	2:L:106:LYS:O	2.07	0.71
1:H:27:TYR:CE1	1:H:98:ARG:HD3	2.25	0.71
2:L:113:PRO:HG2	2:L:136:LEU:CD2	2.19	0.71
2:L:114:THR:O	2:L:135:PHE:N	2.22	0.71
2:L:8:HIS:C	2:L:106:LYS:CA	2.59	0.71
1:H:2:VAL:HG23	1:H:27:TYR:CD2	2.26	0.71
2:L:10:ALA:N	2:L:106:LYS:HZ2	1.88	0.71
1:H:101:THR:HG23	1:H:102:PHE:HB2	1.71	0.71
2:L:115:VAL:HB	2:L:136:LEU:HA	1.73	0.71
2:L:113:PRO:C	2:L:175:MET:C	2.49	0.71
2:L:32:ASN:CB	2:L:33:THR:CA	2.69	0.71
1:H:170:PRO:CD	2:L:162:SER:OG	2.38	0.70
2:L:110:LEU:O	2:L:163:TRP:CD1	2.44	0.70
2:L:53:ASP:OD1	2:L:53:ASP:O	2.09	0.70
2:L:34:VAL:CG2	2:L:67:LYS:HZ1	2.05	0.70
1:H:169:PHE:CG	2:L:176:SER:HB2	2.26	0.70
2:L:48:LEU:O	2:L:56:PRO:CD	2.36	0.70
2:L:105:THR:CG2	2:L:105:THR:O	2.39	0.69
2:L:114:THR:CG2	2:L:135:PHE:CG	2.75	0.69
2:L:67:LYS:HD2	2:L:72:ALA:HB2	1.75	0.69
1:H:136:ASN:O	1:H:188:SER:HB3	1.92	0.68
1:H:9:PRO:HB2	1:H:111:THR:O	1.93	0.68
2:L:53:ASP:HA	2:L:65:ALA:HB3	1.75	0.68
2:L:112:ALA:HB3	2:L:163:TRP:N	2.07	0.68
2:L:40:PHE:CE1	2:L:82:GLU:O	2.46	0.68
2:L:32:ASN:HB2	2:L:33:THR:HA	1.76	0.68
2:L:10:ALA:CA	2:L:106:LYS:NZ	2.56	0.68
2:L:112:ALA:CB	2:L:175:MET:HG3	2.23	0.68
2:L:113:PRO:O	2:L:175:MET:O	2.11	0.67
1:H:159:SER:H	1:H:199:ASN:ND2	1.91	0.67
2:L:66:SER:O	2:L:67:LYS:HG2	1.95	0.67
2:L:9:SER:HA	2:L:106:LYS:HD2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:111:GLY:HA2	2:L:163:TRP:CH2	2.30	0.67
1:H:50:ARG:NH1	2:L:94:ASP:OD1	2.27	0.67
2:L:113:PRO:O	2:L:175:MET:C	2.32	0.66
2:L:114:THR:O	2:L:134:CYS:C	2.33	0.66
2:L:67:LYS:NZ	2:L:72:ALA:HB1	2.10	0.66
1:H:169:PHE:CE2	2:L:175:MET:O	2.49	0.66
1:H:50:ARG:NE	2:L:99:TRP:CZ3	2.63	0.66
2:L:92:TRP:CD1	2:L:94:ASP:HB2	2.29	0.66
1:H:93:VAL:HG22	1:H:111:THR:HG22	1.77	0.66
2:L:52:LYS:O	2:L:65:ALA:HB1	1.96	0.66
2:L:110:LEU:H	2:L:142:LYS:HE3	1.61	0.66
2:L:112:ALA:HA	2:L:163:TRP:CZ3	2.30	0.66
2:L:113:PRO:CG	2:L:136:LEU:HD13	2.26	0.66
2:L:113:PRO:O	2:L:136:LEU:N	2.29	0.66
2:L:111:GLY:CA	2:L:163:TRP:CH2	2.78	0.66
2:L:47:LEU:HD23	2:L:56:PRO:HG2	1.77	0.66
2:L:114:THR:N	2:L:134:CYS:O	2.29	0.65
2:L:67:LYS:HB2	2:L:72:ALA:HA	1.75	0.65
2:L:112:ALA:HB2	2:L:175:MET:CG	2.26	0.65
2:L:113:PRO:HG2	2:L:136:LEU:CB	2.27	0.65
2:L:48:LEU:C	2:L:56:PRO:HG2	2.17	0.65
2:L:67:LYS:CD	2:L:72:ALA:CB	2.73	0.65
2:L:7:PRO:C	2:L:106:LYS:CB	2.64	0.65
2:L:111:GLY:O	2:L:163:TRP:NE1	2.30	0.65
1:H:169:PHE:HE2	2:L:175:MET:CA	2.09	0.65
2:L:18:VAL:CG1	2:L:76:ILE:HD12	2.27	0.65
2:L:10:ALA:N	2:L:106:LYS:NZ	2.45	0.64
2:L:113:PRO:CD	2:L:175:MET:HB3	2.27	0.64
2:L:115:VAL:HG23	2:L:136:LEU:CD1	2.24	0.64
2:L:87:TYR:N	2:L:105:THR:HG21	2.12	0.64
2:L:66:SER:O	2:L:67:LYS:CG	2.45	0.64
1:H:38:LYS:HD3	1:H:94:TYR:CZ	2.31	0.64
2:L:52:LYS:O	2:L:65:ALA:CB	2.46	0.64
2:L:113:PRO:HG3	2:L:175:MET:SD	2.36	0.64
1:H:99:SER:HB3	1:H:103:PHE:CD1	2.31	0.64
2:L:112:ALA:O	2:L:112:ALA:CB	2.44	0.64
2:L:113:PRO:HD2	2:L:136:LEU:HB2	1.80	0.64
2:L:114:THR:N	2:L:136:LEU:HD12	2.12	0.64
2:L:113:PRO:HG2	2:L:136:LEU:HB2	1.80	0.64
2:L:86:ASP:CA	2:L:105:THR:CG2	2.62	0.64
2:L:40:PHE:HE1	2:L:82:GLU:O	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:GLN:NE2	1:H:96:CYS:H	1.96	0.63
2:L:34:VAL:CG1	2:L:67:LYS:HE3	2.20	0.63
2:L:111:GLY:HA3	2:L:163:TRP:CD1	2.33	0.63
2:L:175:MET:C	2:L:175:MET:HG2	2.18	0.63
2:L:9:SER:CB	2:L:106:LYS:O	2.47	0.63
2:L:87:TYR:H	2:L:105:THR:CG2	2.12	0.63
2:L:40:PHE:HA	2:L:85:ALA:CB	2.28	0.63
2:L:92:TRP:HD1	2:L:94:ASP:C	2.02	0.63
2:L:113:PRO:C	2:L:175:MET:O	2.37	0.63
2:L:84:GLU:O	2:L:85:ALA:HB2	1.99	0.62
2:L:32:ASN:CB	2:L:33:THR:HA	2.29	0.62
2:L:7:PRO:CB	2:L:106:LYS:HD3	2.29	0.62
2:L:114:THR:CB	2:L:135:PHE:CD1	2.73	0.62
2:L:34:VAL:HG11	2:L:67:LYS:CE	2.21	0.62
1:H:101:THR:N	1:H:102:PHE:HB3	2.14	0.62
2:L:114:THR:N	2:L:136:LEU:HD13	2.15	0.62
2:L:66:SER:O	2:L:67:LYS:CB	2.47	0.62
1:H:38:LYS:HD2	1:H:92:ALA:HB3	1.82	0.62
2:L:114:THR:CA	2:L:134:CYS:O	2.46	0.62
1:H:20:ILE:CG1	1:H:81:MET:HB3	2.29	0.62
2:L:7:PRO:CG	2:L:106:LYS:CE	2.75	0.62
1:H:27:TYR:CZ	1:H:98:ARG:HD3	2.34	0.62
1:H:36:TRP:CD1	1:H:70:LEU:HD13	2.35	0.61
2:L:114:THR:OG1	2:L:134:CYS:N	2.32	0.61
2:L:66:SER:C	2:L:67:LYS:HG2	2.20	0.61
2:L:7:PRO:CG	2:L:106:LYS:CD	2.78	0.61
2:L:8:HIS:CA	2:L:106:LYS:CB	2.78	0.61
1:H:136:ASN:HA	1:H:188:SER:OG	2.01	0.61
2:L:163:TRP:CD2	2:L:163:TRP:CB	2.73	0.61
2:L:87:TYR:H	2:L:105:THR:HG21	1.66	0.60
2:L:55:ARG:HH12	2:L:61:ASP:CA	2.09	0.60
2:L:67:LYS:CG	2:L:72:ALA:HA	2.31	0.60
2:L:115:VAL:N	2:L:136:LEU:N	2.50	0.60
2:L:110:LEU:N	2:L:142:LYS:CE	2.64	0.60
1:H:169:PHE:CE2	2:L:175:MET:CA	2.84	0.60
2:L:92:TRP:CD1	2:L:94:ASP:N	2.68	0.60
2:L:33:THR:CG2	2:L:95:SER:CB	2.80	0.60
2:L:67:LYS:HD2	2:L:72:ALA:CA	2.32	0.60
2:L:112:ALA:HB1	2:L:162:SER:O	2.02	0.60
2:L:86:ASP:C	2:L:105:THR:HG21	2.22	0.60
2:L:114:THR:C	2:L:136:LEU:N	2.53	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:67:LYS:CD	2:L:72:ALA:HA	2.32	0.60
2:L:113:PRO:CD	2:L:175:MET:CB	2.79	0.59
2:L:114:THR:C	2:L:134:CYS:C	2.61	0.59
2:L:110:LEU:H	2:L:142:LYS:CE	2.14	0.59
2:L:112:ALA:CA	2:L:175:MET:HG2	2.30	0.59
1:H:169:PHE:CZ	2:L:175:MET:O	2.55	0.59
2:L:112:ALA:N	2:L:175:MET:HG3	2.15	0.59
1:H:167:HIS:NE2	2:L:174:SER:OG	2.35	0.59
1:H:32:TYR:CE2	1:H:98:ARG:NH1	2.71	0.58
1:H:2:VAL:HG21	1:H:98:ARG:HH21	1.68	0.58
2:L:14:PRO:O	2:L:15:ASP:HB3	2.03	0.58
1:H:172:VAL:HG12	2:L:160:LEU:HD22	1.82	0.58
2:L:113:PRO:CB	2:L:175:MET:HE2	2.07	0.58
2:L:9:SER:N	2:L:106:LYS:CB	2.52	0.58
2:L:67:LYS:CD	2:L:72:ALA:CA	2.81	0.58
2:L:108:THR:C	2:L:109:VAL:HG13	2.24	0.58
2:L:114:THR:N	2:L:134:CYS:C	2.51	0.58
2:L:92:TRP:HD1	2:L:95:SER:N	2.02	0.58
2:L:111:GLY:O	2:L:112:ALA:CB	2.52	0.57
2:L:113:PRO:C	2:L:136:LEU:CD1	2.70	0.57
2:L:112:ALA:CB	2:L:175:MET:HG2	2.34	0.57
2:L:111:GLY:O	2:L:112:ALA:HB2	2.04	0.57
2:L:7:PRO:CB	2:L:106:LYS:CD	2.82	0.57
2:L:33:THR:HG21	2:L:92:TRP:CB	2.32	0.57
2:L:87:TYR:N	2:L:105:THR:CG2	2.68	0.57
1:H:50:ARG:NH2	2:L:99:TRP:CZ3	2.68	0.57
1:H:38:LYS:HB2	1:H:48:ILE:CD1	2.16	0.57
1:H:6:GLN:HE21	1:H:96:CYS:HB3	1.70	0.57
1:H:20:ILE:HD12	1:H:36:TRP:CZ3	2.40	0.57
2:L:115:VAL:CB	2:L:136:LEU:HA	2.35	0.56
2:L:55:ARG:HH12	2:L:61:ASP:CB	2.18	0.56
1:H:106:TRP:CZ2	2:L:45:PRO:HB2	2.40	0.56
2:L:7:PRO:CD	2:L:106:LYS:HD3	2.36	0.56
2:L:66:SER:O	2:L:67:LYS:HB3	2.04	0.56
2:L:15:ASP:O	2:L:15:ASP:OD1	2.24	0.56
2:L:108:THR:O	2:L:109:VAL:HG13	2.06	0.56
1:H:50:ARG:CG	1:H:59:LYS:HB2	2.30	0.56
1:H:87:THR:OG1	1:H:89:GLU:HG2	2.06	0.56
1:H:187:PRO:HG2	1:H:190:THR:OG1	2.05	0.56
2:L:111:GLY:CA	2:L:111:GLY:C	2.74	0.56
1:H:167:HIS:CE1	2:L:174:SER:OG	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:14:PRO:O	2:L:15:ASP:CB	2.53	0.56
2:L:114:THR:C	2:L:135:PHE:CA	2.75	0.55
2:L:113:PRO:CG	2:L:136:LEU:CD2	2.83	0.55
2:L:33:THR:CG2	2:L:95:SER:OG	2.54	0.55
1:H:169:PHE:CG	2:L:176:SER:CB	2.90	0.55
2:L:47:LEU:CD2	2:L:56:PRO:HG3	2.36	0.55
2:L:111:GLY:O	2:L:175:MET:CG	2.39	0.55
2:L:7:PRO:CD	2:L:106:LYS:CE	2.77	0.55
2:L:106:LYS:C	2:L:107:LEU:CD1	2.67	0.55
1:H:40:LYS:HD2	1:H:43:GLN:OE1	2.06	0.55
2:L:108:THR:O	2:L:109:VAL:CG1	2.55	0.55
2:L:36:TRP:C	2:L:37:TYR:HD1	2.09	0.55
2:L:135:PHE:N	2:L:135:PHE:C	2.54	0.54
2:L:113:PRO:CG	2:L:136:LEU:CG	2.84	0.54
2:L:47:LEU:HD23	2:L:56:PRO:CG	2.38	0.54
2:L:33:THR:HG1	2:L:92:TRP:HB2	1.73	0.54
2:L:7:PRO:CG	2:L:106:LYS:HD3	2.38	0.54
1:H:102:PHE:CD1	2:L:50:TYR:CB	2.86	0.54
2:L:146:VAL:CG2	2:L:175:MET:HE2	2.37	0.54
2:L:163:TRP:CZ2	2:L:175:MET:SD	3.01	0.54
1:H:197:THR:HG22	1:H:212:LYS:HA	1.90	0.54
2:L:33:THR:CB	2:L:92:TRP:HB2	2.37	0.53
1:H:22:CYS:HG	1:H:96:CYS:HG	1.53	0.53
2:L:52:LYS:CD	2:L:67:LYS:O	2.56	0.53
2:L:7:PRO:HB2	2:L:106:LYS:HD2	1.90	0.53
2:L:112:ALA:HB3	2:L:163:TRP:CE3	2.43	0.53
1:H:34:ILE:HD12	1:H:79:ALA:HB2	1.91	0.53
1:H:22:CYS:SG	1:H:96:CYS:SG	3.07	0.53
1:H:102:PHE:HZ	2:L:56:PRO:HG3	1.74	0.53
2:L:114:THR:HG21	2:L:135:PHE:CE1	2.44	0.53
2:L:67:LYS:NZ	2:L:72:ALA:CB	2.71	0.53
1:H:20:ILE:HD11	1:H:81:MET:HB3	1.90	0.52
2:L:112:ALA:C	2:L:175:MET:CE	2.77	0.52
2:L:93:ASP:OD1	2:L:94:ASP:N	2.42	0.52
1:H:12:VAL:HG22	1:H:16:ALA:HB3	1.90	0.52
2:L:87:TYR:HB2	2:L:105:THR:OG1	2.08	0.52
2:L:7:PRO:O	2:L:106:LYS:HD3	2.09	0.52
2:L:34:VAL:HG22	2:L:67:LYS:HZ1	1.74	0.52
1:H:8:GLY:N	1:H:9:PRO:CD	2.73	0.52
1:H:5:GLN:CG	1:H:23:LYS:HB3	2.39	0.52
1:H:51:ILE:HG13	1:H:57:ASN:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:92:TRP:CD1	2:L:94:ASP:CA	2.93	0.52
2:L:8:HIS:O	2:L:107:LEU:N	2.43	0.52
2:L:112:ALA:HB1	2:L:162:SER:H	1.75	0.52
1:H:20:ILE:HG12	1:H:81:MET:HB3	1.90	0.52
2:L:79:LEU:C	2:L:79:LEU:HD23	2.30	0.52
1:H:8:GLY:N	1:H:9:PRO:HD2	2.25	0.52
2:L:84:GLU:O	2:L:85:ALA:CB	2.58	0.51
2:L:112:ALA:N	2:L:163:TRP:CZ3	2.77	0.51
1:H:6:GLN:HE22	1:H:107:GLY:CA	2.08	0.51
1:H:169:PHE:HD2	2:L:162:SER:O	1.93	0.51
2:L:92:TRP:HB3	2:L:95:SER:CB	2.17	0.51
1:H:2:VAL:HG23	1:H:27:TYR:CE2	2.45	0.51
2:L:113:PRO:HB2	2:L:136:LEU:HD11	1.90	0.51
2:L:113:PRO:CD	2:L:136:LEU:HD13	2.34	0.51
2:L:86:ASP:HB3	2:L:105:THR:HG22	1.92	0.51
2:L:105:THR:O	2:L:106:LYS:C	2.49	0.51
2:L:47:LEU:CD2	2:L:56:PRO:CG	2.89	0.51
1:H:5:GLN:HG3	1:H:23:LYS:HB3	1.93	0.51
1:H:12:VAL:HG11	1:H:86:LEU:HD13	1.92	0.51
1:H:124:VAL:O	1:H:211:LYS:HE3	2.10	0.51
2:L:34:VAL:HG13	2:L:52:LYS:HA	1.93	0.50
2:L:8:HIS:C	2:L:106:LYS:HA	2.27	0.50
1:H:129:PRO:HB3	1:H:134:GLN:NE2	2.26	0.50
1:H:170:PRO:HG3	2:L:163:TRP:O	2.11	0.50
2:L:93:ASP:CB	2:L:99:TRP:HE3	2.14	0.50
2:L:115:VAL:CG2	2:L:136:LEU:CG	2.65	0.50
1:H:170:PRO:C	2:L:162:SER:HG	2.13	0.50
2:L:8:HIS:C	2:L:106:LYS:C	2.69	0.50
2:L:112:ALA:N	2:L:175:MET:CG	2.68	0.50
1:H:83:LEU:HB3	1:H:86:LEU:HD21	1.94	0.50
2:L:32:ASN:HB2	2:L:33:THR:OG1	2.08	0.50
1:H:38:LYS:CG	1:H:92:ALA:HB3	2.42	0.50
1:H:33:TYR:CZ	1:H:52:TYR:HB2	2.47	0.50
2:L:107:LEU:O	2:L:108:THR:HG23	2.12	0.50
1:H:134:GLN:O	1:H:134:GLN:HG3	2.12	0.50
2:L:155:ARG:NH2	2:L:185:GLU:OE2	2.45	0.50
2:L:112:ALA:HB3	2:L:162:SER:CA	2.41	0.49
1:H:170:PRO:HD2	2:L:162:SER:OG	2.11	0.49
1:H:102:PHE:CZ	2:L:56:PRO:HG3	2.48	0.49
2:L:7:PRO:C	2:L:106:LYS:CD	2.76	0.49
1:H:27:TYR:CE1	1:H:98:ARG:CD	2.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:10:ALA:HA	2:L:106:LYS:NZ	2.26	0.49
2:L:9:SER:CA	2:L:106:LYS:HG3	2.42	0.49
2:L:9:SER:C	2:L:106:LYS:HG3	2.33	0.49
2:L:8:HIS:N	2:L:106:LYS:HB2	2.28	0.49
2:L:49:ILE:HG21	2:L:65:ALA:CB	2.42	0.49
2:L:113:PRO:CB	2:L:175:MET:SD	2.99	0.49
2:L:7:PRO:HG2	2:L:106:LYS:CD	2.40	0.49
1:H:186:VAL:HB	1:H:187:PRO:HD2	1.94	0.49
1:H:169:PHE:HE2	2:L:175:MET:N	2.10	0.49
2:L:113:PRO:CG	2:L:136:LEU:CD1	2.91	0.49
2:L:114:THR:CG2	2:L:176:SER:HA	2.43	0.49
1:H:169:PHE:CE1	2:L:176:SER:HB2	2.48	0.48
1:H:39:GLN:C	1:H:92:ALA:HB1	2.34	0.48
2:L:8:HIS:CA	2:L:106:LYS:HA	2.42	0.48
1:H:35:ASN:OD1	1:H:50:ARG:CB	2.61	0.48
1:H:40:LYS:CG	1:H:41:PRO:HD2	2.44	0.48
2:L:37:TYR:N	2:L:37:TYR:HD1	2.11	0.48
2:L:112:ALA:CA	2:L:163:TRP:CE3	2.91	0.48
2:L:93:ASP:HA	2:L:99:TRP:CB	2.38	0.48
2:L:7:PRO:HB2	2:L:106:LYS:CD	2.42	0.48
1:H:33:TYR:CE2	1:H:52:TYR:CB	2.96	0.48
2:L:113:PRO:HD2	2:L:175:MET:CG	2.42	0.48
1:H:34:ILE:HD12	1:H:79:ALA:CB	2.44	0.48
2:L:150:ILE:HD11	2:L:179:LEU:HD21	1.95	0.48
1:H:37:MET:SD	1:H:46:GLU:C	2.92	0.48
1:H:127:LEU:HB2	1:H:142:GLY:CA	2.44	0.48
2:L:86:ASP:CB	2:L:105:THR:HG22	2.44	0.47
2:L:175:MET:HB2	2:L:175:MET:HG3	1.37	0.47
2:L:107:LEU:C	2:L:108:THR:HG23	2.35	0.47
1:H:202:HIS:HB3	1:H:207:THR:HB	1.96	0.47
2:L:113:PRO:HA	2:L:177:SER:N	2.29	0.47
2:L:114:THR:CG2	2:L:134:CYS:C	2.83	0.47
1:H:38:LYS:HG2	1:H:92:ALA:HB3	1.97	0.47
1:H:143:CYS:SG	1:H:198:CYS:SG	3.13	0.47
2:L:87:TYR:C	2:L:105:THR:HB	2.31	0.47
1:H:169:PHE:CE2	2:L:176:SER:N	2.83	0.47
1:H:50:ARG:CZ	2:L:99:TRP:CZ3	2.98	0.47
2:L:67:LYS:HB2	2:L:71:SER:C	2.29	0.47
2:L:33:THR:HG22	2:L:95:SER:OG	2.14	0.47
2:L:13:PRO:HG2	2:L:16:GLN:HG3	1.97	0.47
2:L:37:TYR:N	2:L:37:TYR:CD1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:34:VAL:HG13	2:L:34:VAL:O	2.14	0.47
1:H:38:LYS:CD	1:H:92:ALA:HB3	2.44	0.46
1:H:20:ILE:CD1	1:H:81:MET:HB3	2.45	0.46
2:L:186:TYR:CZ	2:L:211:ARG:HD3	2.50	0.46
1:H:100:LEU:HD23	1:H:100:LEU:O	2.16	0.46
2:L:175:MET:CG	2:L:175:MET:HA	2.24	0.46
1:H:101:THR:HG23	1:H:102:PHE:CB	2.44	0.46
1:H:40:LYS:HA	1:H:92:ALA:HB2	1.97	0.46
2:L:7:PRO:HG2	2:L:106:LYS:NZ	2.29	0.46
1:H:40:LYS:HB3	1:H:43:GLN:OE1	2.15	0.46
1:H:8:GLY:H	1:H:9:PRO:HD2	1.81	0.46
1:H:170:PRO:CD	2:L:163:TRP:O	2.64	0.46
2:L:113:PRO:HB3	2:L:175:MET:SD	2.55	0.46
2:L:38:GLN:HB3	2:L:48:LEU:HD11	1.96	0.46
2:L:38:GLN:NE2	2:L:40:PHE:HE2	2.13	0.46
1:H:50:ARG:NH1	2:L:94:ASP:CG	2.69	0.46
1:H:106:TRP:CE3	2:L:45:PRO:HD2	2.51	0.46
2:L:109:VAL:HB	2:L:142:LYS:HD3	1.97	0.46
1:H:38:LYS:HG2	1:H:92:ALA:CB	2.46	0.46
2:L:52:LYS:HG3	2:L:67:LYS:HG2	1.97	0.45
1:H:38:LYS:CD	1:H:94:TYR:CZ	2.99	0.45
1:H:136:ASN:CG	1:H:137:SER:H	2.20	0.45
2:L:112:ALA:N	2:L:163:TRP:CH2	2.81	0.45
2:L:86:ASP:CB	2:L:105:THR:CG2	2.94	0.45
2:L:61:ASP:OD1	2:L:61:ASP:O	2.34	0.45
1:H:4:LEU:HD21	1:H:27:TYR:OH	2.17	0.45
2:L:114:THR:HG22	2:L:176:SER:HA	1.98	0.45
2:L:107:LEU:O	2:L:108:THR:CG2	2.65	0.45
2:L:51:GLY:O	2:L:52:LYS:HB3	2.16	0.45
1:H:170:PRO:O	2:L:162:SER:OG	2.19	0.44
2:L:92:TRP:CD1	2:L:94:ASP:CB	2.99	0.44
2:L:93:ASP:CB	2:L:99:TRP:HB3	2.48	0.44
2:L:111:GLY:CA	2:L:163:TRP:CZ3	3.00	0.44
1:H:102:PHE:HD1	2:L:35:ASN:OD1	2.00	0.44
1:H:147:GLY:HA2	1:H:177:LEU:HB3	1.99	0.44
2:L:115:VAL:N	2:L:136:LEU:HG	2.32	0.44
2:L:115:VAL:N	2:L:136:LEU:CA	2.80	0.44
2:L:67:LYS:HD3	2:L:72:ALA:CA	2.47	0.44
1:H:40:LYS:HG3	1:H:41:PRO:HD2	2.00	0.44
2:L:38:GLN:OE1	2:L:48:LEU:HD21	2.16	0.44
2:L:52:LYS:O	2:L:65:ALA:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:67:LYS:HZ3	2:L:72:ALA:CB	2.21	0.44
1:H:32:TYR:CZ	1:H:98:ARG:NH1	2.86	0.44
1:H:126:PRO:HD3	1:H:211:LYS:HG2	1.99	0.44
2:L:113:PRO:N	2:L:175:MET:CB	2.79	0.44
1:H:181:SER:HG	2:L:176:SER:HG	1.62	0.44
1:H:50:ARG:CZ	2:L:99:TRP:CE3	2.96	0.44
1:H:195:THR:HG22	1:H:197:THR:HG23	1.99	0.44
1:H:6:GLN:HE21	1:H:96:CYS:CB	2.31	0.44
1:H:6:GLN:NE2	1:H:96:CYS:HB3	2.33	0.44
1:H:180:LEU:HD12	1:H:180:LEU:C	2.38	0.44
1:H:101:THR:CG2	1:H:102:PHE:HB2	2.43	0.43
1:H:169:PHE:CD2	2:L:162:SER:O	2.70	0.43
1:H:38:LYS:HZ3	1:H:64:PHE:HZ	1.66	0.43
2:L:114:THR:HG1	2:L:114:THR:CB	2.18	0.43
2:L:85:ALA:O	2:L:107:LEU:CD2	2.60	0.43
1:H:98:ARG:O	1:H:104:ASP:OD1	2.36	0.43
1:H:9:PRO:C	1:H:10:GLU:HG2	2.39	0.43
1:H:172:VAL:HG21	2:L:160:LEU:HB3	2.01	0.43
1:H:22:CYS:HB3	1:H:79:ALA:HB3	1.99	0.43
1:H:33:TYR:CD2	1:H:52:TYR:HB2	2.53	0.43
2:L:92:TRP:NE1	2:L:94:ASP:CB	2.62	0.43
2:L:163:TRP:CE2	2:L:175:MET:SD	3.12	0.43
2:L:113:PRO:CB	2:L:175:MET:CE	2.71	0.43
2:L:47:LEU:HD23	2:L:47:LEU:C	2.39	0.43
2:L:7:PRO:N	2:L:106:LYS:HD3	2.34	0.42
1:H:136:ASN:HA	1:H:188:SER:CB	2.49	0.42
1:H:68:ALA:HA	1:H:82:GLN:O	2.19	0.42
2:L:9:SER:C	2:L:106:LYS:O	2.57	0.42
2:L:115:VAL:N	2:L:136:LEU:HA	2.35	0.42
2:L:146:VAL:HG21	2:L:175:MET:CE	2.43	0.42
2:L:92:TRP:CD1	2:L:94:ASP:C	2.89	0.42
2:L:17:THR:CG2	2:L:77:SER:O	2.53	0.42
2:L:59:VAL:HA	2:L:60:PRO:HD3	1.85	0.42
1:H:141:LEU:HD22	1:H:213:ILE:HG21	2.01	0.42
2:L:113:PRO:O	2:L:113:PRO:HD2	2.18	0.42
2:L:115:VAL:O	2:L:115:VAL:HG12	2.18	0.42
2:L:93:ASP:N	2:L:99:TRP:HB3	2.33	0.42
2:L:112:ALA:CB	2:L:163:TRP:N	2.74	0.42
2:L:101:PHE:CD1	2:L:101:PHE:N	2.87	0.42
1:H:33:TYR:CE1	1:H:53:PRO:HD2	2.54	0.42
1:H:12:VAL:O	1:H:114:VAL:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:TYR:CG	1:H:98:ARG:HD2	2.54	0.42
2:L:108:THR:C	2:L:109:VAL:CG1	2.88	0.42
2:L:67:LYS:CD	2:L:72:ALA:HB1	2.48	0.42
2:L:7:PRO:CD	2:L:106:LYS:CD	2.97	0.42
2:L:67:LYS:HD3	2:L:72:ALA:HA	2.02	0.41
1:H:33:TYR:CD2	1:H:52:TYR:CB	3.03	0.41
2:L:112:ALA:CA	2:L:163:TRP:CD2	2.89	0.41
2:L:19:THR:HG22	2:L:75:THR:HG22	2.01	0.41
2:L:13:PRO:HG2	2:L:16:GLN:CG	2.51	0.41
1:H:170:PRO:CG	2:L:163:TRP:O	2.68	0.41
1:H:148:TYR:CE2	1:H:153:VAL:HG13	2.54	0.41
2:L:175:MET:HA	2:L:175:MET:HG2	1.85	0.41
2:L:113:PRO:N	2:L:175:MET:CE	2.83	0.41
2:L:35:ASN:CB	2:L:37:TYR:HE1	2.34	0.41
1:H:167:HIS:CD2	2:L:174:SER:OG	2.72	0.41
1:H:2:VAL:HG21	1:H:105:VAL:HG21	2.03	0.41
2:L:112:ALA:HB2	2:L:163:TRP:HA	2.02	0.40
1:H:70:LEU:HD13	1:H:81:MET:HE1	2.03	0.40
2:L:113:PRO:O	2:L:136:LEU:HB2	2.22	0.40
2:L:32:ASN:CB	2:L:33:THR:CB	2.62	0.40
1:H:2:VAL:HG23	1:H:27:TYR:HD2	1.83	0.40
1:H:136:ASN:C	1:H:188:SER:HB3	2.41	0.40
1:H:106:TRP:CD1	2:L:45:PRO:O	2.75	0.40
2:L:111:GLY:CA	2:L:163:TRP:CE3	2.76	0.40
2:L:163:TRP:NE1	2:L:163:TRP:CD2	2.87	0.40
2:L:97:ASN:HA	2:L:98:GLY:HA2	1.80	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 PDB entries followed by that with respect to all EM entries.

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	H	215/217 (99%)	203 (94%)	9 (4%)	3 (1%)	14 58
2	L	203/205 (99%)	181 (89%)	14 (7%)	8 (4%)	4 36
All	All	418/422 (99%)	384 (92%)	23 (6%)	11 (3%)	11 45

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	10	GLU
1	H	102	PHE
1	H	137	SER
2	L	67	LYS
2	L	85	ALA
2	L	106	LYS
2	L	109	VAL
2	L	116	SER
2	L	32	ASN
2	L	103	GLY
2	L	15	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	H	187/187 (100%)	185 (99%)	2 (1%)	80 91
2	L	177/177 (100%)	174 (98%)	3 (2%)	68 87
All	All	364/364 (100%)	359 (99%)	5 (1%)	76 89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	65	LYS
1	H	162	LEU
2	L	113	PRO
2	L	114	THR
2	L	136	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	6	GLN
1	H	77	ASN
1	H	134	GLN
1	H	199	ASN
2	L	32	ASN
2	L	124	GLN
2	L	190	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.