wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:51 PM BST

PDB ID	:	3J7E
EMDB ID:	:	EMD-5994
Title	:	Electron cryo-microscopy of human papillomavirus 16 and H16.V5 Fab fragments
Authors	:	Lee, H.; Brendle, S.A.; Bywaters, S.M.; Christensen, N.D.; Hafenstein, S.
Deposited on	:	2014-06-23
Resolution	:	13.60 Å(reported)
Based on PDB ID	:	?

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

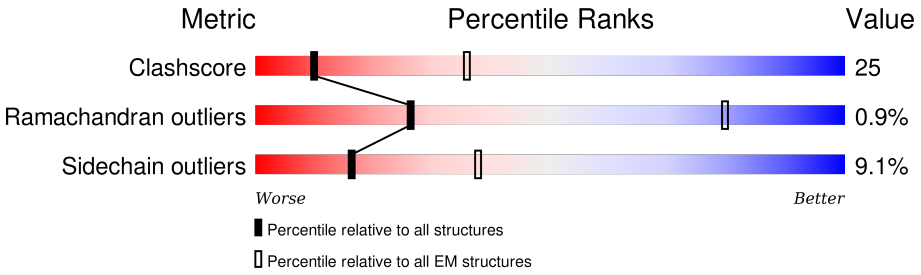
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 13.60 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	A	115	66% 26% 5% •
1	C	115	65% 27% 5% •
1	E	115	66% 26% 5% •
1	L	115	65% 27% 5% •
2	B	121	67% 25% 6% •
2	D	121	65% 26% 6% •
2	F	121	66% 26% 5% •
2	H	121	67% 26% 5% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7356 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 H16.V5 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	115	Total	C	N	O	S	0	0
			885	554	149	177	5		
1	A	115	Total	C	N	O	S	0	0
			885	554	149	177	5		
1	C	115	Total	C	N	O	S	0	0
			885	554	149	177	5		
1	E	115	Total	C	N	O	S	0	0
			885	554	149	177	5		

- Molecule 2 is a protein called H16.V5 Fab heavy chain.

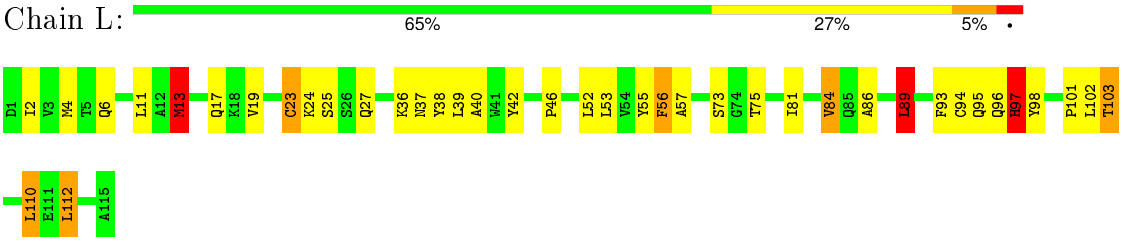
Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	121	Total	C	N	O	S	0	0
			954	614	150	186	4		
2	B	121	Total	C	N	O	S	0	0
			954	614	150	186	4		
2	D	121	Total	C	N	O	S	0	0
			954	614	150	186	4		
2	F	121	Total	C	N	O	S	0	0
			954	614	150	186	4		

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.

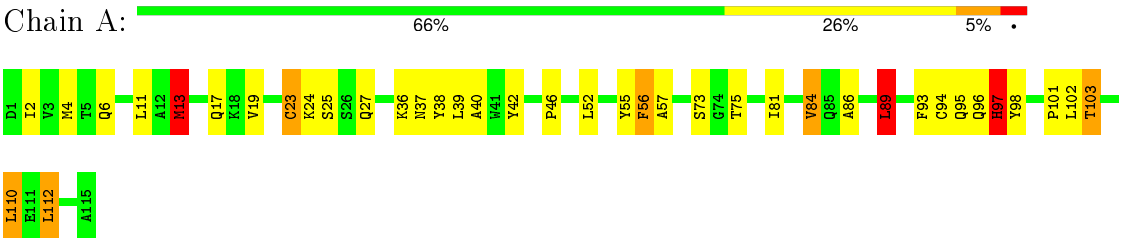
- Molecule 1: H16.V5 Fab light chain

Chain L:



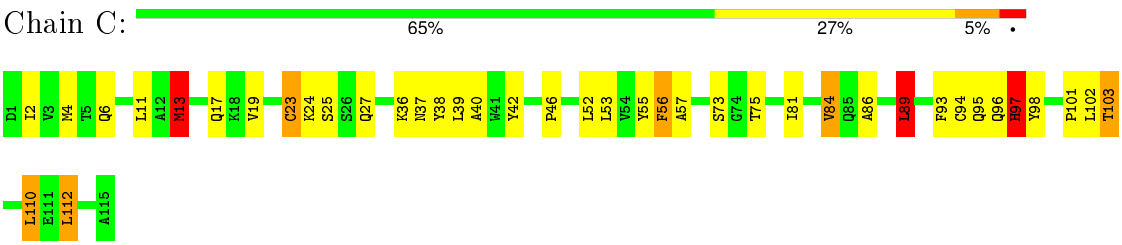
- Molecule 1: H16.V5 Fab light chain

Chain A:



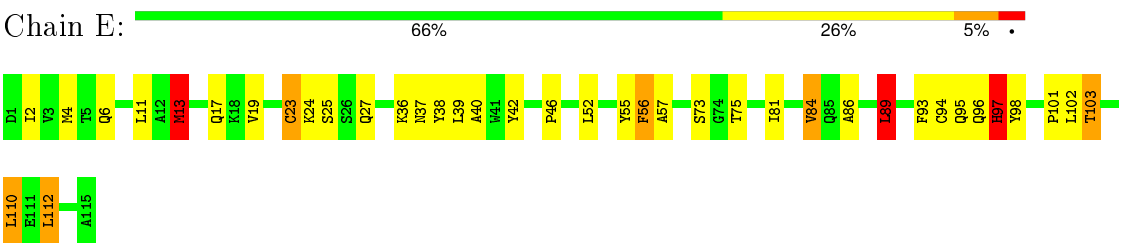
- Molecule 1: H16.V5 Fab light chain

Chain C:



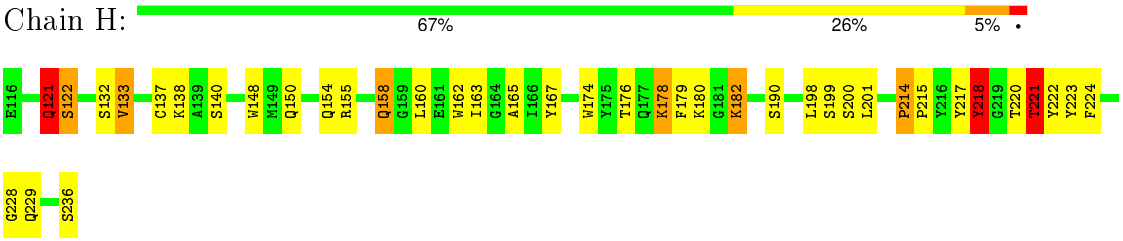
- Molecule 1: H16.V5 Fab light chain

Chain E:



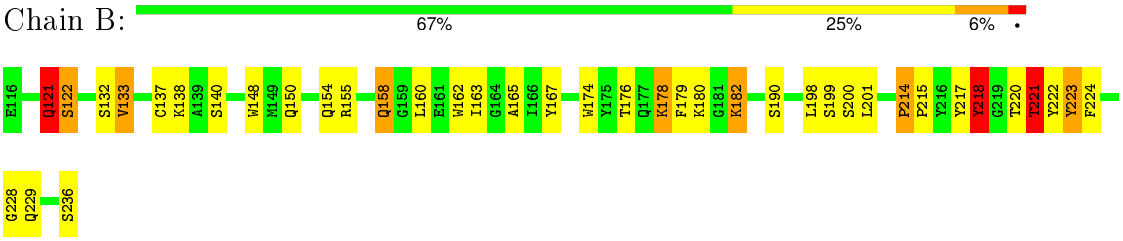
- Molecule 2: H16.V5 Fab heavy chain

Chain H:



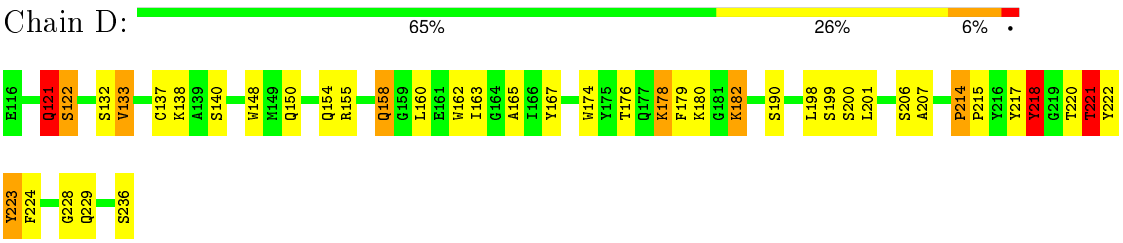
- Molecule 2: H16.V5 Fab heavy chain

Chain B:



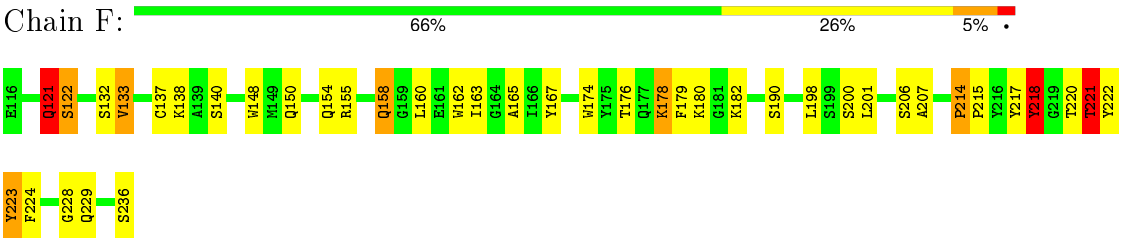
- Molecule 2: H16.V5 Fab heavy chain

Chain D:



- Molecule 2: H16.V5 Fab heavy chain

Chain F:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	2075	Depositor
Resolution determination method	FSC 0.5	Depositor
CTF correction method	Each particle	Depositor
Microscope	JEOL 2100	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	690	Depositor
Maximum defocus (nm)	3990	Depositor
Magnification	80000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	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	A	0.94	0/902	1.56	11/1217 (0.9%)
1	C	0.94	0/902	1.55	12/1217 (1.0%)
1	E	0.94	0/902	1.56	11/1217 (0.9%)
1	L	0.94	0/902	1.56	12/1217 (1.0%)
2	B	1.33	2/984 (0.2%)	1.24	10/1337 (0.7%)
2	D	1.33	3/984 (0.3%)	1.24	10/1337 (0.7%)
2	F	1.33	2/984 (0.2%)	1.24	9/1337 (0.7%)
2	H	1.33	2/984 (0.2%)	1.24	9/1337 (0.7%)
All	All	1.16	9/7544 (0.1%)	1.40	84/10216 (0.8%)

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	A	0	1
1	C	0	1
1	E	0	1
1	L	0	1
2	B	0	2
2	D	0	2
2	F	0	2
2	H	0	2
All	All	0	12

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	229	GLN	CD-OE1	7.77	1.41	1.24
2	H	229	GLN	CD-OE1	7.75	1.41	1.24
2	F	229	GLN	CD-OE1	7.74	1.41	1.24
2	D	229	GLN	CD-OE1	7.74	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	122	SER	C-O	-6.59	1.10	1.23
2	H	122	SER	C-O	-6.57	1.10	1.23
2	F	122	SER	C-O	-6.56	1.10	1.23
2	D	122	SER	C-O	-6.50	1.11	1.23
2	D	174	TRP	CD2-CE2	-5.02	1.35	1.41

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	13	MET	CG-SD-CE	-24.75	60.60	100.20
1	L	13	MET	CG-SD-CE	-24.75	60.61	100.20
1	A	13	MET	CG-SD-CE	-24.74	60.61	100.20
1	E	13	MET	CG-SD-CE	-24.71	60.66	100.20
1	C	84	VAL	CG1-CB-CG2	14.09	133.44	110.90
1	E	84	VAL	CG1-CB-CG2	14.03	133.34	110.90
1	L	84	VAL	CG1-CB-CG2	14.00	133.31	110.90
1	A	84	VAL	CG1-CB-CG2	14.00	133.30	110.90
2	F	121	GLN	O-C-N	-13.16	101.64	122.70
2	H	121	GLN	O-C-N	-13.11	101.73	122.70
2	D	121	GLN	O-C-N	-13.10	101.74	122.70
2	B	121	GLN	O-C-N	-13.08	101.77	122.70
1	E	84	VAL	CA-CB-CG2	-10.00	95.90	110.90
1	L	84	VAL	CA-CB-CG2	-9.99	95.92	110.90
1	C	84	VAL	CA-CB-CG2	-9.97	95.94	110.90
1	A	84	VAL	CA-CB-CG2	-9.93	96.00	110.90
1	L	84	VAL	CA-CB-CG1	-8.20	98.61	110.90
1	A	84	VAL	CA-CB-CG1	-8.15	98.68	110.90
1	E	84	VAL	CA-CB-CG1	-8.14	98.69	110.90
1	C	84	VAL	CA-CB-CG1	-8.10	98.75	110.90
2	H	221	THR	CA-CB-CG2	7.49	122.88	112.40
2	B	221	THR	CA-CB-CG2	7.49	122.88	112.40
2	D	221	THR	CA-CB-CG2	7.47	122.86	112.40
2	F	221	THR	CA-CB-CG2	7.46	122.85	112.40
1	A	112	LEU	N-CA-CB	-7.02	96.35	110.40
1	E	112	LEU	N-CA-CB	-7.01	96.37	110.40
1	C	112	LEU	N-CA-CB	-7.01	96.38	110.40
1	L	112	LEU	N-CA-CB	-7.01	96.39	110.40
1	A	112	LEU	CA-CB-CG	-6.85	99.54	115.30
1	L	112	LEU	CA-CB-CG	-6.82	99.61	115.30
1	C	112	LEU	CA-CB-CG	-6.80	99.66	115.30
1	E	112	LEU	CA-CB-CG	-6.80	99.66	115.30
2	F	121	GLN	CA-C-N	6.49	131.47	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	121	GLN	CA-C-N	6.42	131.33	117.20
2	D	121	GLN	CA-C-N	6.42	131.33	117.20
2	B	121	GLN	CA-C-N	6.41	131.29	117.20
2	F	229	GLN	OE1-CD-NE2	-6.33	107.33	121.90
2	H	229	GLN	OE1-CD-NE2	-6.33	107.35	121.90
2	B	229	GLN	OE1-CD-NE2	-6.33	107.35	121.90
2	H	229	GLN	CG-CD-NE2	6.31	131.84	116.70
2	B	229	GLN	CG-CD-NE2	6.30	131.82	116.70
2	D	229	GLN	OE1-CD-NE2	-6.30	107.41	121.90
2	D	229	GLN	CG-CD-NE2	6.26	131.73	116.70
1	E	56	PHE	CB-CG-CD2	-6.26	116.42	120.80
1	L	56	PHE	CB-CG-CD2	-6.23	116.44	120.80
2	F	229	GLN	CG-CD-NE2	6.23	131.65	116.70
1	A	56	PHE	CB-CG-CD2	-6.21	116.45	120.80
1	C	56	PHE	CB-CG-CD2	-6.20	116.46	120.80
1	C	103	THR	CA-CB-CG2	6.18	121.05	112.40
1	L	103	THR	CA-CB-CG2	6.15	121.01	112.40
1	A	97	HIS	CG-ND1-CE1	-6.15	97.70	105.70
1	A	103	THR	CA-CB-CG2	6.15	121.01	112.40
1	E	97	HIS	CG-ND1-CE1	-6.14	97.71	105.70
1	L	97	HIS	CG-ND1-CE1	-6.14	97.72	105.70
1	E	103	THR	CA-CB-CG2	6.09	120.93	112.40
1	C	97	HIS	CG-ND1-CE1	-6.07	97.81	105.70
1	A	97	HIS	ND1-CE1-NE2	5.51	122.03	109.90
1	L	97	HIS	ND1-CE1-NE2	5.46	121.91	109.90
1	E	97	HIS	ND1-CE1-NE2	5.45	121.88	109.90
1	C	97	HIS	ND1-CE1-NE2	5.43	121.84	109.90
2	H	148	TRP	CD1-NE1-CE2	-5.32	104.21	109.00
2	D	223	TYR	CB-CG-CD1	-5.27	117.84	121.00
2	B	174	TRP	CD1-NE1-CE2	-5.21	104.31	109.00
2	F	148	TRP	CD1-NE1-CE2	-5.21	104.31	109.00
2	B	223	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	B	148	TRP	CD1-NE1-CE2	-5.17	104.35	109.00
2	D	174	TRP	CD1-NE1-CE2	-5.16	104.35	109.00
2	F	174	TRP	CD1-NE1-CE2	-5.16	104.35	109.00
2	F	223	TYR	CB-CG-CD1	-5.15	117.91	121.00
2	D	148	TRP	CD1-NE1-CE2	-5.14	104.37	109.00
2	D	174	TRP	CG-CD2-CE3	-5.14	129.28	133.90
2	B	218	TYR	N-CA-CB	5.12	119.82	110.60
2	H	174	TRP	CD1-NE1-CE2	-5.11	104.40	109.00
2	H	174	TRP	CG-CD2-CE3	-5.10	129.31	133.90
2	D	218	TYR	N-CA-CB	5.05	119.70	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	218	TYR	N-CA-CB	5.05	119.69	110.60
2	H	218	TYR	N-CA-CB	5.05	119.69	110.60
2	B	174	TRP	CG-CD2-CE3	-5.05	129.36	133.90
1	L	89	LEU	CA-CB-CG	5.03	126.88	115.30
1	E	89	LEU	CA-CB-CG	5.03	126.88	115.30
1	C	89	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	89	LEU	CA-CB-CG	5.01	126.82	115.30
1	C	53	LEU	CB-CA-C	-5.01	100.68	110.20
1	L	53	LEU	CB-CA-C	-5.01	100.69	110.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	HIS	Sidechain
2	B	121	GLN	Mainchain
2	B	122	SER	Mainchain
1	C	97	HIS	Sidechain
2	D	121	GLN	Mainchain
2	D	122	SER	Mainchain
1	E	97	HIS	Sidechain
2	F	121	GLN	Mainchain
2	F	122	SER	Mainchain
2	H	121	GLN	Mainchain
2	H	122	SER	Mainchain
1	L	97	HIS	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	885	0	873	60	0
1	C	885	0	873	61	0
1	E	885	0	873	63	0
1	L	885	0	873	64	0
2	B	954	0	898	48	0
2	D	954	0	898	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	954	0	898	51	0
2	H	954	0	898	48	0
All	All	7356	0	7084	359	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 25.

All (359) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:MET:SD	1:E:19:VAL:HG13	1.94	1.08
1:L:13:MET:SD	1:L:19:VAL:HG13	1.94	1.07
1:C:13:MET:SD	1:C:19:VAL:HG13	1.94	1.07
1:A:13:MET:SD	1:A:19:VAL:HG13	1.95	1.07
1:L:86:ALA:HA	1:L:112:LEU:HD11	1.44	1.00
1:C:86:ALA:HA	1:C:112:LEU:HD11	1.44	0.99
1:E:86:ALA:HA	1:E:112:LEU:HD11	1.44	0.99
1:A:86:ALA:HA	1:A:112:LEU:HD11	1.44	0.99
1:A:36:LYS:HB3	2:B:220:THR:HB	1.51	0.92
1:E:36:LYS:HB3	2:F:220:THR:HB	1.51	0.92
1:C:36:LYS:HB3	2:D:220:THR:HB	1.51	0.91
1:L:36:LYS:HB3	2:H:220:THR:HB	1.51	0.91
1:A:101:PRO:HA	2:B:162:TRP:CZ3	2.09	0.88
1:E:101:PRO:HA	2:F:162:TRP:CZ3	2.09	0.88
1:L:101:PRO:HA	2:H:162:TRP:CZ3	2.09	0.87
1:C:101:PRO:HA	2:D:162:TRP:CZ3	2.09	0.87
1:A:38:TYR:HA	2:B:221:THR:HB	1.58	0.85
1:L:38:TYR:HA	2:H:221:THR:HB	1.59	0.84
1:E:38:TYR:HA	2:F:221:THR:HB	1.58	0.84
1:C:13:MET:SD	1:C:19:VAL:CG1	2.66	0.84
1:L:13:MET:SD	1:L:19:VAL:CG1	2.66	0.84
1:E:13:MET:SD	1:E:19:VAL:CG1	2.66	0.83
1:A:13:MET:SD	1:A:19:VAL:CG1	2.66	0.83
1:C:38:TYR:HA	2:D:221:THR:HB	1.58	0.82
2:D:163:ILE:O	2:D:176:THR:HG22	1.86	0.76
1:C:56:PHE:HB2	2:D:220:THR:HG21	1.66	0.76
1:E:56:PHE:HB2	2:F:220:THR:HG21	1.66	0.76
2:H:215:PRO:HD2	2:H:223:TYR:O	1.86	0.76
1:A:56:PHE:HB2	2:B:220:THR:HG21	1.66	0.76
2:F:163:ILE:O	2:F:176:THR:HG22	1.85	0.76
2:B:215:PRO:HD2	2:B:223:TYR:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:PRO:HD2	2:D:223:TYR:O	1.86	0.76
1:E:86:ALA:HA	1:E:112:LEU:CD1	2.16	0.76
1:L:56:PHE:HB2	2:H:220:THR:HG21	1.66	0.75
2:H:163:ILE:O	2:H:176:THR:HG22	1.85	0.75
1:L:86:ALA:HA	1:L:112:LEU:CD1	2.16	0.74
1:C:86:ALA:HA	1:C:112:LEU:CD1	2.16	0.74
1:A:86:ALA:HA	1:A:112:LEU:CD1	2.16	0.74
2:B:163:ILE:O	2:B:176:THR:HG22	1.85	0.74
2:F:215:PRO:HD2	2:F:223:TYR:O	1.86	0.74
1:C:96:GLN:HG2	1:C:103:THR:H	1.53	0.73
1:E:97:HIS:HB2	2:F:221:THR:OG1	1.88	0.73
1:L:96:GLN:HG2	1:L:103:THR:H	1.53	0.73
1:C:56:PHE:CB	2:D:220:THR:HG21	2.19	0.72
1:L:97:HIS:HB2	2:H:221:THR:OG1	1.88	0.72
2:B:221:THR:HG23	2:B:223:TYR:HB3	1.71	0.72
1:L:56:PHE:CB	2:H:220:THR:HG21	2.20	0.72
1:A:97:HIS:HB2	2:B:221:THR:OG1	1.88	0.72
1:E:96:GLN:HG2	1:E:103:THR:H	1.53	0.72
2:D:221:THR:HG23	2:D:223:TYR:HB3	1.71	0.72
1:C:97:HIS:HB2	2:D:221:THR:OG1	1.88	0.72
1:A:56:PHE:CB	2:B:220:THR:HG21	2.19	0.71
1:E:56:PHE:CB	2:F:220:THR:HG21	2.19	0.71
2:H:221:THR:HG23	2:H:223:TYR:HB3	1.71	0.71
1:A:96:GLN:HG2	1:A:103:THR:H	1.53	0.71
2:F:221:THR:HG23	2:F:223:TYR:HB3	1.71	0.70
1:E:2:ILE:HB	1:E:96:GLN:NE2	2.11	0.65
1:L:2:ILE:HB	1:L:96:GLN:NE2	2.11	0.65
1:A:81:ILE:CG2	1:A:84:VAL:HG22	2.26	0.65
1:C:2:ILE:HB	1:C:96:GLN:NE2	2.11	0.65
1:E:81:ILE:CG2	1:E:84:VAL:HG22	2.27	0.65
1:E:38:TYR:CE1	2:F:220:THR:HA	2.31	0.65
1:C:38:TYR:CE1	2:D:220:THR:HA	2.31	0.65
1:L:38:TYR:CE1	2:H:220:THR:HA	2.31	0.65
1:C:81:ILE:CG2	1:C:84:VAL:HG22	2.26	0.65
1:L:81:ILE:CG2	1:L:84:VAL:HG22	2.27	0.64
1:A:2:ILE:HB	1:A:96:GLN:NE2	2.11	0.64
1:A:38:TYR:CE1	2:B:220:THR:HA	2.31	0.64
1:E:52:LEU:HD21	2:F:223:TYR:HD1	1.63	0.64
1:C:52:LEU:HD21	2:D:223:TYR:HD1	1.63	0.64
1:L:52:LEU:HD21	2:H:223:TYR:HD1	1.62	0.63
1:A:52:LEU:HD21	2:B:223:TYR:HD1	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:GLN:HG3	2:B:224:PHE:HE1	1.64	0.63
1:L:13:MET:CE	1:L:84:VAL:HG11	2.29	0.63
2:H:150:GLN:HG3	2:H:224:PHE:HE1	1.64	0.63
1:E:13:MET:CE	1:E:84:VAL:HG11	2.29	0.63
2:H:176:THR:CG2	2:H:179:PHE:HD1	2.12	0.63
1:A:13:MET:CE	1:A:84:VAL:HG11	2.29	0.63
2:F:150:GLN:HG3	2:F:224:PHE:HE1	1.64	0.63
2:B:176:THR:CG2	2:B:179:PHE:HD1	2.12	0.63
1:C:13:MET:CE	1:C:84:VAL:HG11	2.29	0.63
2:D:176:THR:CG2	2:D:179:PHE:HD1	2.12	0.63
2:F:176:THR:CG2	2:F:179:PHE:HD1	2.12	0.62
2:D:150:GLN:HG3	2:D:224:PHE:HE1	1.64	0.62
2:D:176:THR:HG21	2:D:179:PHE:HD1	1.65	0.62
2:F:176:THR:HG21	2:F:179:PHE:HD1	1.65	0.62
2:H:176:THR:HG21	2:H:179:PHE:HD1	1.65	0.61
2:B:176:THR:HG21	2:B:179:PHE:HD1	1.65	0.61
1:C:17:GLN:O	1:C:84:VAL:HG23	2.00	0.61
1:L:17:GLN:O	1:L:84:VAL:HG23	2.01	0.61
1:A:17:GLN:O	1:A:84:VAL:HG23	2.01	0.61
1:E:17:GLN:O	1:E:84:VAL:HG23	2.01	0.61
1:A:97:HIS:HB3	2:B:222:TYR:HB2	1.82	0.60
1:C:97:HIS:HB3	2:D:222:TYR:HB2	1.82	0.60
1:L:97:HIS:HB3	2:H:222:TYR:HB2	1.82	0.60
1:A:36:LYS:CB	2:B:220:THR:HB	2.30	0.59
1:E:97:HIS:HB3	2:F:222:TYR:HB2	1.83	0.59
1:E:13:MET:HE3	1:E:84:VAL:HG11	1.86	0.58
1:C:13:MET:CE	1:C:110:LEU:HD21	2.34	0.58
1:A:13:MET:CE	1:A:110:LEU:HD21	2.34	0.57
2:B:178:LYS:O	2:B:178:LYS:HD3	2.04	0.57
2:H:150:GLN:HG3	2:H:224:PHE:CE1	2.40	0.57
2:D:178:LYS:O	2:D:178:LYS:HD3	2.04	0.57
2:F:178:LYS:O	2:F:178:LYS:HD3	2.04	0.57
1:L:13:MET:CE	1:L:110:LEU:HD21	2.34	0.57
1:C:38:TYR:CD2	2:D:221:THR:HA	2.40	0.57
1:A:38:TYR:CD2	2:B:221:THR:HA	2.40	0.57
1:L:38:TYR:CD2	2:H:221:THR:HA	2.40	0.57
2:H:178:LYS:O	2:H:178:LYS:HD3	2.04	0.57
2:F:150:GLN:HG3	2:F:224:PHE:CE1	2.40	0.56
1:E:13:MET:CE	1:E:110:LEU:HD21	2.34	0.56
2:B:150:GLN:HG3	2:B:224:PHE:CE1	2.40	0.56
2:D:150:GLN:HG3	2:D:224:PHE:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:LYS:CB	2:H:220:THR:HB	2.30	0.56
2:F:150:GLN:OE1	2:F:165:ALA:HB2	2.06	0.56
2:B:150:GLN:OE1	2:B:165:ALA:HB2	2.06	0.56
2:D:150:GLN:OE1	2:D:165:ALA:HB2	2.06	0.56
2:H:150:GLN:OE1	2:H:165:ALA:HB2	2.06	0.56
1:E:38:TYR:CD2	2:F:221:THR:HA	2.40	0.55
1:C:13:MET:SD	1:C:84:VAL:HB	2.47	0.55
1:L:13:MET:SD	1:L:84:VAL:HB	2.47	0.55
1:L:13:MET:HE3	1:L:84:VAL:HG11	1.89	0.55
1:C:13:MET:HE3	1:C:84:VAL:HG11	1.89	0.55
1:A:13:MET:SD	1:A:84:VAL:HB	2.47	0.54
1:E:13:MET:SD	1:E:84:VAL:HB	2.47	0.54
1:A:23:CYS:HG	1:A:94:CYS:CB	2.20	0.54
1:A:6:GLN:HE22	1:A:93:PHE:HA	1.72	0.54
1:C:6:GLN:HE22	1:C:93:PHE:HA	1.72	0.53
1:C:36:LYS:CB	2:D:220:THR:HB	2.30	0.53
1:E:6:GLN:HE22	1:E:93:PHE:HA	1.73	0.53
1:C:46:PRO:HG2	1:C:89:LEU:HD13	1.91	0.53
1:A:13:MET:HE3	1:A:84:VAL:HG11	1.90	0.53
1:A:13:MET:HE1	1:A:84:VAL:HG11	1.91	0.53
1:C:23:CYS:HG	1:C:94:CYS:CB	2.21	0.53
1:E:36:LYS:CB	2:F:220:THR:HB	2.30	0.52
1:L:6:GLN:HE22	1:L:93:PHE:HA	1.72	0.52
2:D:133:VAL:HG22	2:D:201:LEU:HD11	1.92	0.52
2:F:133:VAL:HG22	2:F:201:LEU:HD11	1.92	0.52
1:L:101:PRO:CA	2:H:162:TRP:CZ3	2.89	0.52
2:H:198:LEU:HB3	2:H:201:LEU:HD21	1.91	0.52
2:F:214:PRO:HB2	2:F:222:TYR:HD2	1.75	0.52
1:L:46:PRO:HG2	1:L:89:LEU:HD13	1.91	0.52
1:A:46:PRO:HG2	1:A:89:LEU:HD13	1.92	0.52
1:E:13:MET:HE1	1:E:110:LEU:HD21	1.91	0.52
1:E:101:PRO:CA	2:F:162:TRP:CZ3	2.88	0.52
1:E:86:ALA:CA	1:E:112:LEU:HD11	2.31	0.51
1:L:56:PHE:CG	2:H:220:THR:HG21	2.45	0.51
2:D:214:PRO:HB2	2:D:222:TYR:HD2	1.75	0.51
1:A:2:ILE:HB	1:A:96:GLN:HE22	1.75	0.51
2:H:214:PRO:HB2	2:H:222:TYR:HD2	1.75	0.51
2:H:133:VAL:HG22	2:H:201:LEU:HD11	1.91	0.51
2:D:198:LEU:HB3	2:D:201:LEU:HD21	1.91	0.51
1:C:56:PHE:CG	2:D:220:THR:HG21	2.45	0.51
2:F:198:LEU:HB3	2:F:201:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:VAL:HG22	2:B:201:LEU:HD11	1.91	0.51
1:A:56:PHE:CG	2:B:220:THR:HG21	2.45	0.51
2:B:214:PRO:HB2	2:B:222:TYR:HD2	1.75	0.51
1:E:56:PHE:CG	2:F:220:THR:HG21	2.45	0.51
1:E:46:PRO:HG2	1:E:89:LEU:HD13	1.92	0.51
1:A:52:LEU:CD2	2:B:223:TYR:HD1	2.23	0.51
1:C:95:GLN:HG3	1:C:103:THR:O	2.11	0.51
1:C:101:PRO:CA	2:D:162:TRP:CZ3	2.89	0.51
2:B:198:LEU:HB3	2:B:201:LEU:HD21	1.91	0.51
1:C:13:MET:HE1	1:C:84:VAL:HG11	1.93	0.50
1:A:95:GLN:HG3	1:A:103:THR:O	2.11	0.50
1:L:95:GLN:HG3	1:L:103:THR:O	2.11	0.50
1:A:2:ILE:HG12	1:A:27:GLN:HB2	1.94	0.50
1:E:95:GLN:HG3	1:E:103:THR:O	2.11	0.50
1:C:13:MET:SD	1:C:84:VAL:HG21	2.52	0.50
1:E:38:TYR:CZ	2:F:220:THR:HA	2.47	0.50
1:E:13:MET:SD	1:E:84:VAL:HG21	2.52	0.50
1:L:13:MET:SD	1:L:84:VAL:HG21	2.52	0.50
1:E:52:LEU:CD2	2:F:223:TYR:HD1	2.23	0.50
1:C:2:ILE:HB	1:C:96:GLN:HE22	1.75	0.50
1:L:38:TYR:CZ	2:H:220:THR:HA	2.47	0.50
1:E:23:CYS:HG	1:E:94:CYS:CB	2.21	0.50
1:A:38:TYR:CZ	2:B:220:THR:HA	2.47	0.49
1:A:101:PRO:CA	2:B:162:TRP:CZ3	2.89	0.49
1:L:42:TYR:OH	1:L:97:HIS:HE1	1.95	0.49
1:A:13:MET:SD	1:A:84:VAL:HG21	2.52	0.49
1:L:37:ASN:ND2	1:L:73:SER:HA	2.28	0.49
1:L:13:MET:HE1	1:L:84:VAL:HG11	1.93	0.49
1:C:52:LEU:CD2	2:D:223:TYR:HD1	2.23	0.49
1:L:52:LEU:CD2	2:H:223:TYR:HD1	2.23	0.49
1:E:37:ASN:ND2	1:E:73:SER:HA	2.28	0.49
1:E:2:ILE:HG12	1:E:27:GLN:HB2	1.94	0.49
1:E:42:TYR:OH	1:E:97:HIS:HE1	1.95	0.49
1:C:2:ILE:HG12	1:C:27:GLN:HB2	1.94	0.49
2:B:215:PRO:HG2	2:B:223:TYR:CZ	2.48	0.49
1:C:42:TYR:OH	1:C:97:HIS:HE1	1.95	0.49
1:L:2:ILE:HB	1:L:96:GLN:HE22	1.75	0.49
2:F:215:PRO:HG2	2:F:223:TYR:CZ	2.48	0.49
2:D:215:PRO:HG2	2:D:223:TYR:CZ	2.48	0.49
2:B:215:PRO:O	2:B:222:TYR:HA	2.13	0.49
1:C:38:TYR:CZ	2:D:220:THR:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:ILE:HG12	1:L:27:GLN:HB2	1.94	0.49
2:H:154:GLN:HB2	2:H:160:LEU:HD23	1.95	0.49
1:C:37:ASN:ND2	1:C:73:SER:HA	2.28	0.49
2:H:215:PRO:HG2	2:H:223:TYR:CZ	2.48	0.48
1:E:2:ILE:HB	1:E:96:GLN:HE22	1.75	0.48
1:C:13:MET:HE1	1:C:110:LEU:HD21	1.94	0.48
1:C:86:ALA:CA	1:C:112:LEU:HD11	2.31	0.48
1:A:52:LEU:HD22	2:B:224:PHE:O	2.13	0.48
1:C:52:LEU:HD22	2:D:224:PHE:O	2.13	0.48
1:L:56:PHE:H	2:H:221:THR:HG22	1.79	0.48
2:D:154:GLN:HB2	2:D:160:LEU:HD23	1.95	0.48
1:A:42:TYR:OH	1:A:97:HIS:HE1	1.96	0.48
1:E:56:PHE:H	2:F:221:THR:HG22	1.79	0.48
1:A:37:ASN:ND2	1:A:73:SER:HA	2.27	0.48
2:F:215:PRO:O	2:F:222:TYR:HA	2.13	0.48
2:B:154:GLN:HB2	2:B:160:LEU:HD23	1.95	0.48
1:L:4:MET:SD	1:L:25:SER:HB3	2.54	0.48
1:L:13:MET:HE1	1:L:110:LEU:HD21	1.94	0.48
2:D:215:PRO:O	2:D:222:TYR:HA	2.13	0.48
2:B:155:ARG:H	2:B:158:GLN:NE2	2.12	0.48
1:E:13:MET:HE1	1:E:84:VAL:HG11	1.96	0.48
1:E:36:LYS:HA	1:E:56:PHE:CE1	2.49	0.48
1:L:52:LEU:HD22	2:H:224:PHE:O	2.13	0.48
2:F:154:GLN:HB2	2:F:160:LEU:HD23	1.95	0.48
2:F:155:ARG:H	2:F:158:GLN:NE2	2.12	0.48
1:A:4:MET:SD	1:A:25:SER:HB3	2.54	0.48
2:H:155:ARG:H	2:H:158:GLN:NE2	2.12	0.47
2:D:155:ARG:H	2:D:158:GLN:NE2	2.12	0.47
2:B:121:GLN:HE21	2:B:228:GLY:HA3	1.79	0.47
1:A:13:MET:HE1	1:A:110:LEU:HD21	1.96	0.47
2:H:215:PRO:O	2:H:222:TYR:HA	2.13	0.47
1:L:36:LYS:HA	1:L:56:PHE:CE1	2.49	0.47
1:E:4:MET:SD	1:E:25:SER:HB3	2.54	0.47
1:C:19:VAL:HG22	1:C:81:ILE:HB	1.96	0.47
1:C:4:MET:SD	1:C:25:SER:HB3	2.54	0.47
1:C:36:LYS:HA	1:C:56:PHE:CE1	2.49	0.47
1:E:52:LEU:HD22	2:F:224:PHE:O	2.13	0.47
1:C:56:PHE:H	2:D:221:THR:HG22	1.79	0.47
2:D:121:GLN:HE21	2:D:228:GLY:HA3	1.79	0.47
1:L:19:VAL:HG22	1:L:81:ILE:HB	1.96	0.47
2:H:121:GLN:HE21	2:H:228:GLY:HA3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ALA:CA	1:A:112:LEU:HD11	2.31	0.47
1:A:56:PHE:H	2:B:221:THR:HG22	1.79	0.47
1:A:19:VAL:HG22	1:A:81:ILE:HB	1.96	0.47
2:F:121:GLN:HE21	2:F:228:GLY:HA3	1.79	0.47
2:H:132:SER:HB2	2:H:198:LEU:O	2.16	0.46
2:B:132:SER:HB2	2:B:198:LEU:O	2.16	0.46
1:C:38:TYR:HA	2:D:221:THR:CB	2.39	0.46
2:F:132:SER:HB2	2:F:198:LEU:O	2.16	0.46
1:A:36:LYS:HA	1:A:56:PHE:CE1	2.49	0.46
2:F:155:ARG:HH11	2:F:155:ARG:HG2	1.81	0.46
2:H:155:ARG:HB2	2:H:158:GLN:NE2	2.31	0.46
2:D:155:ARG:HG2	2:D:155:ARG:HH11	1.81	0.46
2:D:215:PRO:HG2	2:D:223:TYR:CE1	2.51	0.46
1:E:19:VAL:HG22	1:E:81:ILE:HB	1.96	0.46
2:F:176:THR:HG21	2:F:179:PHE:CD1	2.49	0.46
2:B:155:ARG:HB2	2:B:158:GLN:NE2	2.31	0.46
1:A:40:ALA:HB3	1:A:97:HIS:NE2	2.31	0.46
1:E:40:ALA:HB3	1:E:97:HIS:NE2	2.31	0.46
1:L:40:ALA:HB3	1:L:97:HIS:NE2	2.31	0.46
2:F:215:PRO:HG2	2:F:223:TYR:CE1	2.51	0.46
2:D:155:ARG:HB2	2:D:158:GLN:NE2	2.31	0.46
2:F:155:ARG:HB2	2:F:158:GLN:NE2	2.31	0.46
1:A:13:MET:HE2	1:A:110:LEU:HD21	1.97	0.46
1:C:40:ALA:HB3	1:C:97:HIS:NE2	2.31	0.46
2:B:215:PRO:HG2	2:B:223:TYR:CE1	2.51	0.45
1:E:36:LYS:HB3	2:F:220:THR:CB	2.36	0.45
1:E:42:TYR:OH	1:E:97:HIS:CE1	2.69	0.45
2:H:215:PRO:HG2	2:H:223:TYR:CE1	2.51	0.45
2:H:155:ARG:HH11	2:H:155:ARG:HG2	1.81	0.45
1:L:42:TYR:OH	1:L:97:HIS:CE1	2.69	0.45
2:B:155:ARG:HH11	2:B:155:ARG:HG2	1.81	0.45
2:D:132:SER:HB2	2:D:198:LEU:O	2.16	0.45
1:A:42:TYR:OH	1:A:97:HIS:CE1	2.69	0.45
1:C:42:TYR:OH	1:C:97:HIS:CE1	2.69	0.45
2:B:176:THR:HG21	2:B:179:PHE:CD1	2.49	0.45
1:C:38:TYR:CA	2:D:221:THR:HB	2.41	0.45
1:L:13:MET:HE2	1:L:110:LEU:HD21	1.99	0.45
2:D:176:THR:HG21	2:D:179:PHE:CD1	2.49	0.45
1:L:112:LEU:HD23	1:L:112:LEU:HA	1.75	0.45
1:C:52:LEU:HB2	2:D:224:PHE:O	2.17	0.45
1:E:38:TYR:HA	2:F:221:THR:CB	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TYR:CD2	1:C:98:TYR:HA	2.53	0.44
2:D:214:PRO:HA	2:D:215:PRO:HD2	1.88	0.44
1:E:38:TYR:CD2	1:E:98:TYR:HA	2.53	0.44
1:L:52:LEU:HB2	2:H:224:PHE:O	2.17	0.44
1:E:52:LEU:HB2	2:F:224:PHE:O	2.17	0.44
1:A:52:LEU:HB2	2:B:224:PHE:O	2.17	0.44
2:B:214:PRO:HA	2:B:215:PRO:HD2	1.88	0.44
1:C:13:MET:HE2	1:C:110:LEU:HD21	1.99	0.44
1:L:38:TYR:CD2	1:L:98:TYR:HA	2.53	0.44
1:A:38:TYR:CD2	1:A:98:TYR:HA	2.53	0.43
1:L:81:ILE:HG22	1:L:84:VAL:HG22	2.00	0.43
1:A:38:TYR:HA	2:B:221:THR:CB	2.39	0.43
1:L:23:CYS:HG	1:L:94:CYS:CB	2.25	0.43
1:E:81:ILE:HG22	1:E:84:VAL:HG22	2.00	0.43
1:A:39:LEU:HA	1:A:95:GLN:O	2.18	0.43
1:E:39:LEU:HA	1:E:95:GLN:O	2.18	0.43
2:F:214:PRO:HA	2:F:215:PRO:HD2	1.88	0.43
1:L:39:LEU:HA	1:L:95:GLN:O	2.18	0.43
2:D:221:THR:O	2:D:223:TYR:HD2	2.02	0.43
1:C:39:LEU:HA	1:C:95:GLN:O	2.18	0.42
1:L:36:LYS:HA	1:L:56:PHE:HE1	1.85	0.42
2:H:155:ARG:HG2	2:H:155:ARG:NH1	2.34	0.42
1:A:36:LYS:HA	1:A:56:PHE:HE1	1.85	0.42
2:D:176:THR:CG2	2:D:179:PHE:CD1	2.99	0.42
2:B:217:TYR:O	2:B:218:TYR:HB2	2.20	0.42
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.75	0.42
1:L:96:GLN:O	1:L:102:LEU:HG	2.20	0.42
1:A:37:ASN:HB2	1:A:57:ALA:HB2	2.02	0.42
2:B:155:ARG:NH1	2:B:155:ARG:HG2	2.34	0.42
2:F:217:TYR:O	2:F:218:TYR:HB2	2.20	0.42
1:E:96:GLN:O	1:E:102:LEU:HG	2.20	0.42
1:E:38:TYR:CA	2:F:221:THR:HB	2.41	0.42
1:C:96:GLN:O	1:C:102:LEU:HG	2.20	0.42
1:L:55:TYR:O	1:L:56:PHE:HB3	2.20	0.42
1:E:37:ASN:HB2	1:E:57:ALA:HB2	2.02	0.42
2:F:155:ARG:HG2	2:F:155:ARG:NH1	2.34	0.42
2:D:155:ARG:HG2	2:D:155:ARG:NH1	2.34	0.42
2:H:217:TYR:O	2:H:218:TYR:HB2	2.20	0.42
1:L:36:LYS:HB3	2:H:220:THR:CB	2.36	0.42
1:C:24:LYS:HA	1:C:75:THR:O	2.20	0.42
1:L:24:LYS:HA	1:L:75:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:ALA:CA	1:L:112:LEU:HD11	2.31	0.42
1:A:96:GLN:O	1:A:102:LEU:HG	2.20	0.42
2:F:221:THR:O	2:F:223:TYR:HD2	2.02	0.42
1:C:55:TYR:O	1:C:56:PHE:HB3	2.20	0.41
1:L:84:VAL:H	1:L:84:VAL:HG23	1.58	0.41
2:H:221:THR:O	2:H:223:TYR:HD2	2.02	0.41
1:C:37:ASN:HB2	1:C:57:ALA:HB2	2.02	0.41
1:A:55:TYR:O	1:A:56:PHE:HB3	2.20	0.41
1:C:84:VAL:HG23	1:C:84:VAL:H	1.58	0.41
1:E:55:TYR:O	1:E:56:PHE:HB3	2.20	0.41
1:L:38:TYR:HA	2:H:221:THR:CB	2.40	0.41
1:A:24:LYS:HA	1:A:75:THR:O	2.20	0.41
2:D:217:TYR:O	2:D:218:TYR:HB2	2.19	0.41
1:E:24:LYS:HA	1:E:75:THR:O	2.20	0.41
2:D:182:LYS:HE3	2:D:199:SER:O	2.21	0.41
2:B:221:THR:O	2:B:223:TYR:HD2	2.02	0.41
1:C:55:TYR:HB3	2:D:223:TYR:HB2	2.03	0.41
1:L:52:LEU:HD21	2:H:223:TYR:CD1	2.50	0.41
1:L:97:HIS:HD1	1:L:102:LEU:CD2	2.34	0.41
2:H:182:LYS:HE3	2:H:199:SER:O	2.21	0.41
1:E:55:TYR:HB3	2:F:223:TYR:HB2	2.03	0.41
2:D:206:SER:O	2:D:207:ALA:HB2	2.21	0.41
1:A:84:VAL:HG23	1:A:84:VAL:H	1.58	0.41
1:E:97:HIS:HD1	1:E:102:LEU:CD2	2.34	0.41
1:L:55:TYR:HB3	2:H:223:TYR:HB2	2.03	0.41
1:L:37:ASN:HB2	1:L:57:ALA:HB2	2.02	0.41
1:C:36:LYS:HA	1:C:56:PHE:HE1	1.84	0.41
1:E:13:MET:HE2	1:E:110:LEU:HD21	2.02	0.40
1:E:36:LYS:HA	1:E:56:PHE:HE1	1.84	0.40
1:E:89:LEU:HB2	1:E:112:LEU:HD12	2.04	0.40
1:C:6:GLN:NE2	1:C:94:CYS:H	2.20	0.40
2:H:176:THR:HG21	2:H:179:PHE:CD1	2.49	0.40
2:B:176:THR:CG2	2:B:179:PHE:CD1	2.99	0.40
1:A:36:LYS:HB3	2:B:220:THR:CB	2.36	0.40
1:A:97:HIS:HD1	1:A:102:LEU:CD2	2.34	0.40
1:L:96:GLN:CG	1:L:96:GLN:O	2.70	0.40
2:B:182:LYS:HE3	2:B:199:SER:O	2.21	0.40
1:E:56:PHE:HB2	2:F:220:THR:CG2	2.45	0.40
1:C:97:HIS:HD1	1:C:102:LEU:CD2	2.34	0.40
2:F:176:THR:CG2	2:F:179:PHE:CD1	2.99	0.40
2:F:206:SER:O	2:F:207:ALA:HB2	2.21	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	A	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
1	C	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
1	E	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
1	L	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
2	B	119/121 (98%)	110 (92%)	7 (6%)	2 (2%)	11	55
2	D	119/121 (98%)	110 (92%)	7 (6%)	2 (2%)	11	55
2	F	119/121 (98%)	110 (92%)	7 (6%)	2 (2%)	11	55
2	H	119/121 (98%)	110 (92%)	7 (6%)	2 (2%)	11	55
All	All	928/944 (98%)	864 (93%)	56 (6%)	8 (1%)	26	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	214	PRO
2	B	214	PRO
2	D	214	PRO
2	F	214	PRO
2	H	218	TYR
2	B	218	TYR
2	D	218	TYR
2	F	218	TYR

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	A	100/100 (100%)	95 (95%)	5 (5%)	30	66
1	C	100/100 (100%)	95 (95%)	5 (5%)	30	66
1	E	100/100 (100%)	95 (95%)	5 (5%)	30	66
1	L	100/100 (100%)	95 (95%)	5 (5%)	30	66
2	B	97/97 (100%)	84 (87%)	13 (13%)	5	27
2	D	97/97 (100%)	84 (87%)	13 (13%)	5	27
2	F	97/97 (100%)	84 (87%)	13 (13%)	5	27
2	H	97/97 (100%)	84 (87%)	13 (13%)	5	27
All	All	788/788 (100%)	716 (91%)	72 (9%)	16	43

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	11	LEU
1	L	13	MET
1	L	23	CYS
1	L	89	LEU
1	L	110	LEU
2	H	133	VAL
2	H	137	CYS
2	H	138	LYS
2	H	140	SER
2	H	158	GLN
2	H	167	TYR
2	H	178	LYS
2	H	180	LYS
2	H	182	LYS
2	H	190	SER
2	H	200	SER
2	H	221	THR
2	H	236	SER
1	A	11	LEU
1	A	13	MET
1	A	23	CYS
1	A	89	LEU
1	A	110	LEU
2	B	133	VAL

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Mol	Chain	Res	Type
2	B	137	CYS
2	B	138	LYS
2	B	140	SER
2	B	158	GLN
2	B	167	TYR
2	B	178	LYS
2	B	180	LYS
2	B	182	LYS
2	B	190	SER
2	B	200	SER
2	B	221	THR
2	B	236	SER
1	C	11	LEU
1	C	13	MET
1	C	23	CYS
1	C	89	LEU
1	C	110	LEU
2	D	133	VAL
2	D	137	CYS
2	D	138	LYS
2	D	140	SER
2	D	158	GLN
2	D	167	TYR
2	D	178	LYS
2	D	180	LYS
2	D	182	LYS
2	D	190	SER
2	D	200	SER
2	D	221	THR
2	D	236	SER
1	E	11	LEU
1	E	13	MET
1	E	23	CYS
1	E	89	LEU
1	E	110	LEU
2	F	133	VAL
2	F	137	CYS
2	F	138	LYS
2	F	140	SER
2	F	158	GLN
2	F	167	TYR
2	F	178	LYS

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Mol	Chain	Res	Type
2	F	180	LYS
2	F	182	LYS
2	F	190	SER
2	F	200	SER
2	F	221	THR
2	F	236	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	96	GLN
1	L	97	HIS
2	H	121	GLN
2	H	158	GLN
1	A	6	GLN
1	A	96	GLN
1	A	97	HIS
2	B	121	GLN
2	B	158	GLN
2	B	229	GLN
1	C	6	GLN
1	C	96	GLN
1	C	97	HIS
2	D	121	GLN
2	D	158	GLN
2	D	229	GLN
1	E	6	GLN
1	E	96	GLN
1	E	97	HIS
2	F	121	GLN
2	F	158	GLN
2	F	229	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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.