



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:50 PM BST

PDB ID : 3J7G
EMDB ID: : EMD-5994
Title : Electron cryo-microscopy of human papillomavirus 16 and H16.V5 Fab fragments
Authors : Lee, H.; Hafenstein, S.
Deposited on : 2014-06-24
Resolution : 13.60 Å(reported)
Based on PDB ID : 3OAE

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

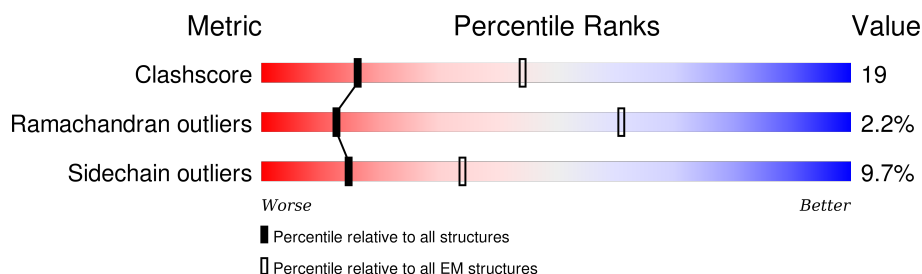
1 Overall quality at a glance ⓘ

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	455	55% 31% 6% 7%
1	B	455	56% 30% 6% 7%
1	C	455	56% 30% 6% 7%
1	D	455	55% 31% 6% 7%
1	E	455	57% 30% 6% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16610 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 L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
1	B	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
1	C	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
1	D	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		
1	E	421	Total	C	N	O	S	0	0
			3322	2116	556	630	20		

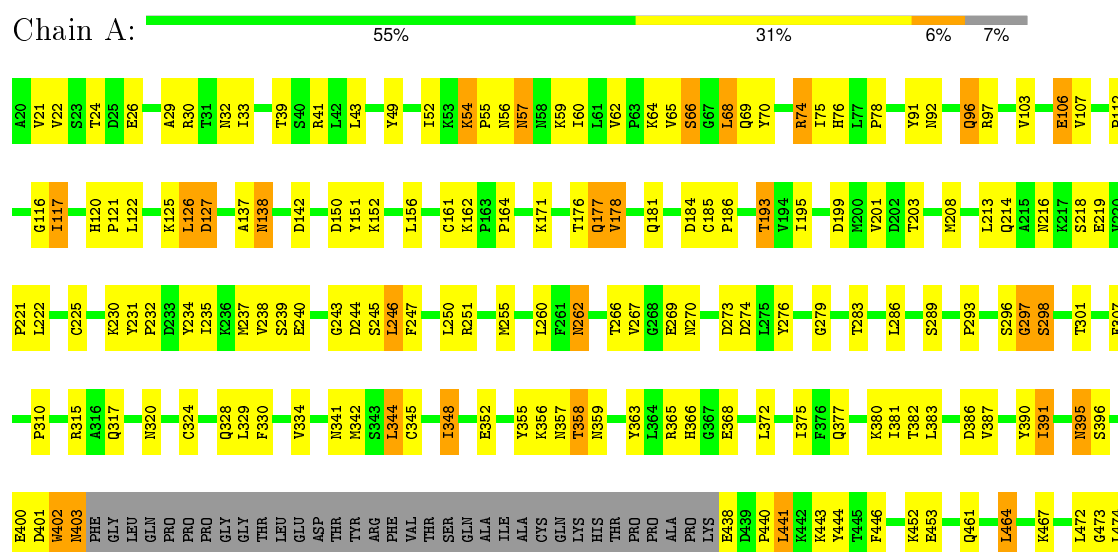
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	EXPRESSION TAG	UNP Q4VRM0
A	177	GLN	ASN	CONFLICT	UNP Q4VRM0
A	181	GLN	ASN	CONFLICT	UNP Q4VRM0
A	472	LEU	ALA	CONFLICT	UNP Q4VRM0
B	20	ALA	-	EXPRESSION TAG	UNP Q4VRM0
B	177	GLN	ASN	CONFLICT	UNP Q4VRM0
B	181	GLN	ASN	CONFLICT	UNP Q4VRM0
B	472	LEU	ALA	CONFLICT	UNP Q4VRM0
C	20	ALA	-	EXPRESSION TAG	UNP Q4VRM0
C	177	GLN	ASN	CONFLICT	UNP Q4VRM0
C	181	GLN	ASN	CONFLICT	UNP Q4VRM0
C	472	LEU	ALA	CONFLICT	UNP Q4VRM0
D	20	ALA	-	EXPRESSION TAG	UNP Q4VRM0
D	177	GLN	ASN	CONFLICT	UNP Q4VRM0
D	181	GLN	ASN	CONFLICT	UNP Q4VRM0
D	472	LEU	ALA	CONFLICT	UNP Q4VRM0
E	20	ALA	-	EXPRESSION TAG	UNP Q4VRM0
E	177	GLN	ASN	CONFLICT	UNP Q4VRM0
E	181	GLN	ASN	CONFLICT	UNP Q4VRM0
E	472	LEU	ALA	CONFLICT	UNP Q4VRM0

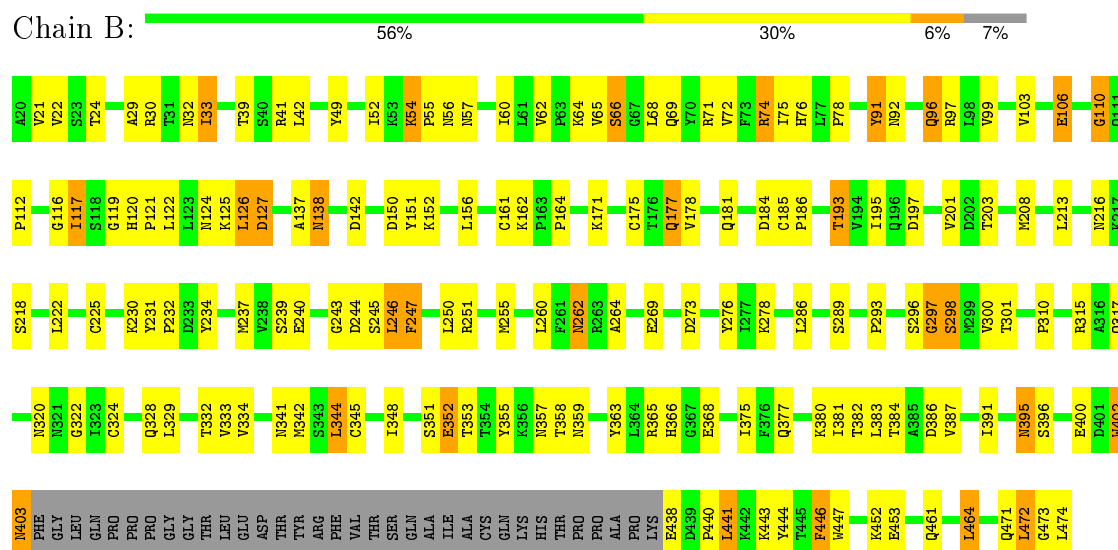
3 Residue-property plots

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. 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: L1

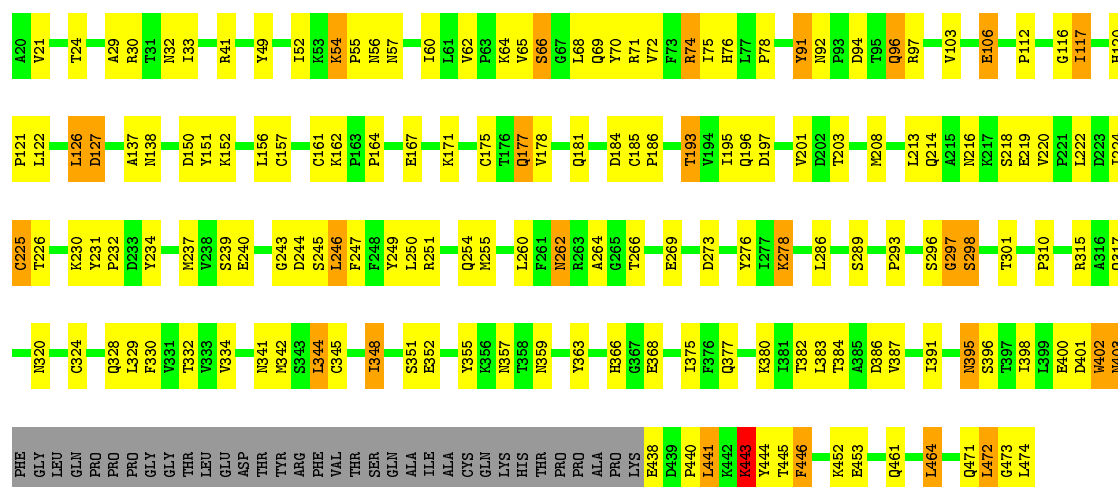


• Molecule 1: L1



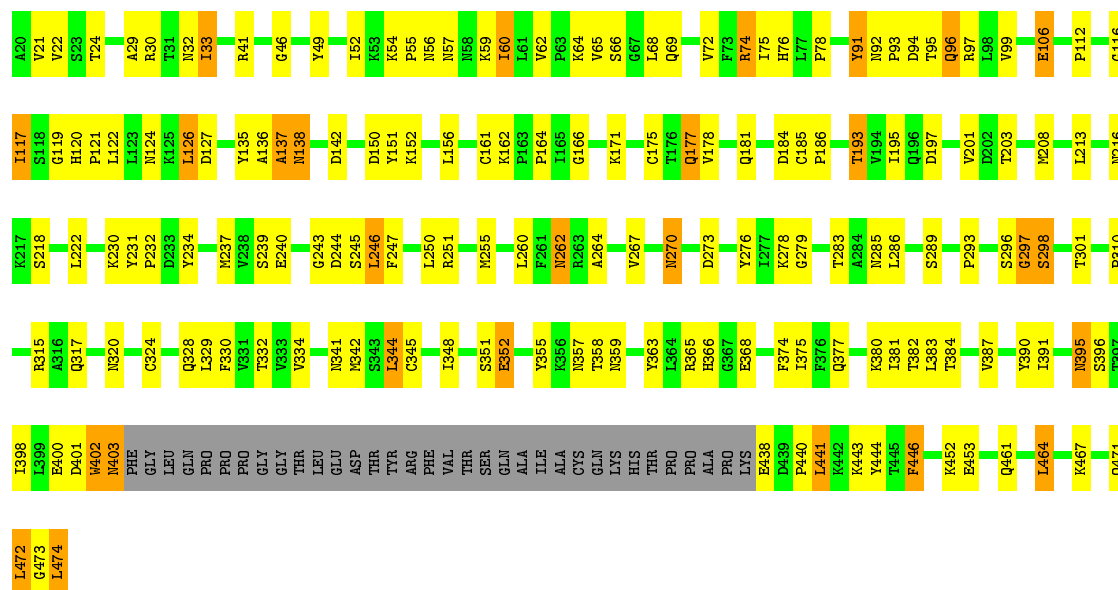
• Molecule 1: L1





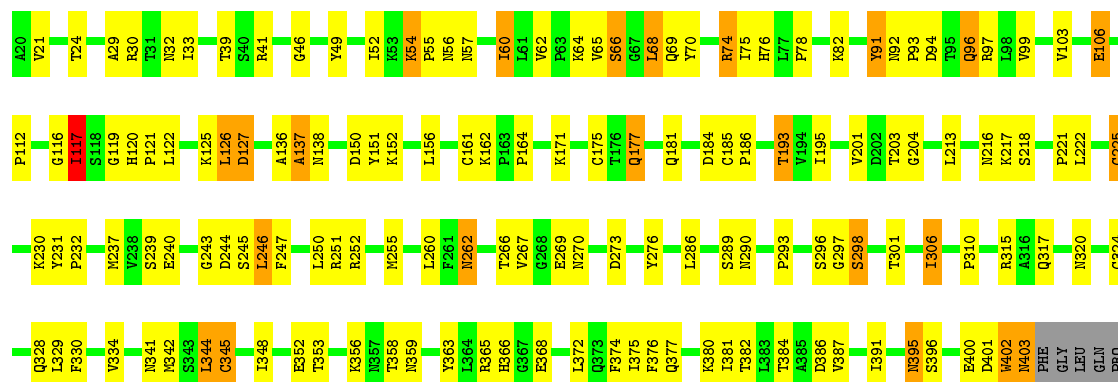
- Molecule 1: L1

Chain D: 55% 31% 6% 7%



- Molecule 1: L1

Chain E: 57% 30% 6% 7%



PRO	PRO	GLY	THR	LEU	GLU	ASP	THR	TYR	ARG	PHE	VAL	THR	SER	GLN	ALA	ILE	ALA	CYS	GLN	LYS	HIS	THR	PRO	PRO	ALA	PRO	LYS	E438	D438	P440	L441	K442	K443	Y444	T445	F446	K452	E453	Q461	L464	Q471	L472	G473	L474
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4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.58	6/3407 (0.2%)	0.72	3/4632 (0.1%)
1	B	0.49	0/3407	0.70	2/4632 (0.0%)
1	C	0.53	2/3407 (0.1%)	0.71	1/4632 (0.0%)
1	D	0.55	3/3407 (0.1%)	0.71	3/4632 (0.1%)
1	E	0.53	1/3407 (0.0%)	0.72	0/4632
All	All	0.54	12/17035 (0.1%)	0.71	9/23160 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	59	LYS	CB-CG	-8.88	1.28	1.52
1	A	443	LYS	CD-CE	-6.57	1.34	1.51
1	A	57	ASN	CG-OD1	-6.33	1.10	1.24
1	C	443	LYS	CD-CE	-6.02	1.36	1.51
1	D	285	ASN	CG-OD1	-6.01	1.10	1.24
1	D	285	ASN	CG-ND2	-5.97	1.18	1.32
1	A	54	LYS	CD-CE	-5.70	1.37	1.51
1	A	443	LYS	CB-CG	-5.59	1.37	1.52
1	C	443	LYS	CG-CD	-5.57	1.33	1.52
1	E	225	CYS	CB-SG	-5.57	1.72	1.81
1	A	443	LYS	CG-CD	-5.42	1.34	1.52
1	A	54	LYS	CE-NZ	-5.16	1.36	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	LYS	CD-CE-NZ	-6.44	96.89	111.70
1	C	297	GLY	N-CA-C	-5.74	98.75	113.10
1	D	297	GLY	N-CA-C	-5.69	98.88	113.10
1	D	59	LYS	CA-CB-CG	5.62	125.76	113.40
1	A	391	ILE	CG1-CB-CG2	-5.55	99.18	111.40
1	A	297	GLY	N-CA-C	-5.47	99.41	113.10
1	B	297	GLY	N-CA-C	-5.34	99.75	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	GLY	N-CA-C	5.25	126.22	113.10
1	D	59	LYS	CB-CA-C	-5.16	100.08	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3227	132	0
1	B	3322	0	3227	141	0
1	C	3322	0	3227	135	0
1	D	3322	0	3227	138	0
1	E	3322	0	3227	135	0
All	All	16610	0	16135	609	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 19.

All (609) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LYS:HB3	1:A:57:ASN:HB3	1.23	1.09
1:C:97:ARG:HH21	1:C:403:ASN:HB2	1.13	1.07
1:B:461:GLN:HE22	1:C:21:VAL:H	1.04	1.01
1:C:54:LYS:HB3	1:C:57:ASN:HB3	1.40	1.01
1:D:461:GLN:HE22	1:E:21:VAL:H	1.05	1.01
1:E:175:CYS:HB3	1:E:177:GLN:OE1	1.61	1.00
1:A:461:GLN:HE22	1:B:21:VAL:H	1.09	0.99
1:A:21:VAL:H	1:E:461:GLN:HE22	1.10	0.96
1:A:97:ARG:HH21	1:A:403:ASN:HB2	1.31	0.94
1:B:54:LYS:HB3	1:B:57:ASN:HB3	1.47	0.93
1:D:121:PRO:HD3	1:D:222:LEU:HD21	1.51	0.92
1:C:461:GLN:HE22	1:D:21:VAL:H	1.10	0.91
1:B:97:ARG:HH21	1:B:403:ASN:HB2	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ALA:HB3	1:E:380:LYS:HG3	1.54	0.87
1:D:443:LYS:HA	1:D:443:LYS:HE2	1.57	0.87
1:B:29:ALA:HB3	1:B:380:LYS:HG3	1.55	0.86
1:B:345:CYS:SG	1:C:216:ASN:HB2	2.14	0.86
1:B:121:PRO:HD3	1:B:222:LEU:HD21	1.58	0.85
1:A:121:PRO:HD3	1:A:222:LEU:HD21	1.58	0.85
1:A:29:ALA:HB3	1:A:380:LYS:HG3	1.58	0.85
1:A:216:ASN:HB2	1:E:345:CYS:SG	2.17	0.84
1:C:121:PRO:HD3	1:C:222:LEU:HD21	1.58	0.84
1:C:345:CYS:SG	1:D:216:ASN:HB2	2.17	0.83
1:C:121:PRO:HG3	1:D:289:SER:HB3	1.59	0.83
1:E:121:PRO:HD3	1:E:222:LEU:HD21	1.58	0.83
1:C:29:ALA:HB3	1:C:380:LYS:HG3	1.60	0.82
1:D:29:ALA:HB3	1:D:380:LYS:HG3	1.59	0.82
1:A:345:CYS:SG	1:B:216:ASN:HB2	2.19	0.82
1:B:443:LYS:HE2	1:B:443:LYS:HA	1.58	0.82
1:A:121:PRO:HG3	1:B:289:SER:HB3	1.62	0.82
1:C:97:ARG:NH2	1:C:403:ASN:HB2	1.95	0.81
1:B:461:GLN:NE2	1:C:21:VAL:H	1.79	0.81
1:E:443:LYS:HE2	1:E:443:LYS:HA	1.62	0.79
1:A:54:LYS:HB3	1:A:57:ASN:CB	2.10	0.79
1:D:97:ARG:HH21	1:D:403:ASN:HB2	1.47	0.79
1:C:461:GLN:NE2	1:D:21:VAL:H	1.80	0.78
1:D:461:GLN:NE2	1:E:21:VAL:H	1.82	0.77
1:D:345:CYS:SG	1:E:216:ASN:HB2	2.24	0.77
1:B:121:PRO:HG3	1:C:289:SER:HB3	1.66	0.76
1:A:289:SER:HB3	1:E:121:PRO:HG3	1.66	0.76
1:A:461:GLN:NE2	1:B:21:VAL:H	1.84	0.76
1:A:21:VAL:H	1:E:461:GLN:NE2	1.83	0.75
1:D:440:PRO:HG2	1:D:441:LEU:HD12	1.68	0.75
1:D:54:LYS:HB3	1:D:57:ASN:CB	2.17	0.75
1:A:366:HIS:HE1	1:A:368:GLU:OE1	1.69	0.74
1:D:121:PRO:HG3	1:E:289:SER:HB3	1.70	0.73
1:D:54:LYS:HB3	1:D:57:ASN:HB3	1.70	0.73
1:D:162:LYS:HB2	1:D:245:SER:HA	1.71	0.73
1:A:162:LYS:HB2	1:A:245:SER:HA	1.71	0.71
1:C:122:LEU:O	1:C:218:SER:HB3	1.90	0.71
1:C:162:LYS:HB2	1:C:245:SER:HA	1.72	0.71
1:B:387:VAL:O	1:B:391:ILE:HD13	1.90	0.71
1:D:122:LEU:O	1:D:218:SER:HB3	1.90	0.71
1:B:402:TRP:O	1:B:403:ASN:C	2.28	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:LYS:HB3	1:C:443:LYS:HZ2	1.56	0.70
1:E:78:PRO:HD3	1:E:452:LYS:HA	1.74	0.70
1:B:152:LYS:HB2	1:B:255:MET:HB2	1.72	0.69
1:E:162:LYS:HB2	1:E:245:SER:HA	1.74	0.69
1:A:122:LEU:O	1:A:218:SER:HB3	1.93	0.69
1:D:152:LYS:HB2	1:D:255:MET:HB2	1.74	0.69
1:D:78:PRO:HD3	1:D:452:LYS:HA	1.75	0.69
1:E:97:ARG:HH21	1:E:403:ASN:HB2	1.58	0.68
1:C:152:LYS:HB2	1:C:255:MET:HB2	1.75	0.68
1:E:152:LYS:HB2	1:E:255:MET:HB2	1.73	0.68
1:E:122:LEU:O	1:E:218:SER:HB3	1.92	0.68
1:B:440:PRO:HG2	1:B:441:LEU:HD12	1.76	0.68
1:B:122:LEU:O	1:B:218:SER:HB3	1.94	0.68
1:B:162:LYS:HB2	1:B:245:SER:HA	1.76	0.68
1:A:176:THR:O	1:A:177:GLN:HG3	1.94	0.67
1:A:78:PRO:HD3	1:A:452:LYS:HA	1.76	0.67
1:E:440:PRO:HG2	1:E:441:LEU:HD12	1.76	0.67
1:B:117:ILE:HG21	1:C:293:PRO:HD3	1.77	0.67
1:A:440:PRO:HG2	1:A:441:LEU:HD12	1.77	0.67
1:C:440:PRO:HG2	1:C:441:LEU:HD12	1.77	0.67
1:B:78:PRO:HD3	1:B:452:LYS:HA	1.78	0.66
1:A:402:TRP:O	1:A:403:ASN:C	2.34	0.66
1:D:68:LEU:HD22	1:D:203:THR:HG22	1.77	0.66
1:B:52:ILE:HB	1:B:62:VAL:HB	1.78	0.66
1:C:117:ILE:HG21	1:D:293:PRO:HD3	1.77	0.65
1:D:402:TRP:O	1:D:403:ASN:C	2.33	0.65
1:D:267:VAL:HG11	1:D:270:ASN:ND2	2.12	0.65
1:B:396:SER:O	1:B:400:GLU:HG3	1.97	0.65
1:C:175:CYS:HB3	1:C:177:GLN:OE1	1.96	0.65
1:C:363:TYR:CE2	1:D:185:CYS:HB2	2.32	0.65
1:C:396:SER:O	1:C:400:GLU:HG3	1.97	0.65
1:A:152:LYS:HB2	1:A:255:MET:HB2	1.76	0.64
1:A:348:ILE:HG22	1:A:359:ASN:OD1	1.97	0.64
1:C:52:ILE:HB	1:C:62:VAL:HB	1.78	0.64
1:C:402:TRP:O	1:C:403:ASN:C	2.34	0.64
1:C:66:SER:H	1:C:69:GLN:NE2	1.95	0.64
1:B:375:ILE:HG12	1:B:464:LEU:HD13	1.80	0.64
1:E:348:ILE:HG22	1:E:359:ASN:OD1	1.96	0.64
1:E:375:ILE:HG12	1:E:464:LEU:HD13	1.78	0.64
1:D:66:SER:H	1:D:69:GLN:NE2	1.95	0.64
1:D:126:LEU:HB3	1:D:262:ASN:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:GLN:HB2	1:E:184:ASP:OD1	1.98	0.63
1:D:375:ILE:HG12	1:D:464:LEU:HD13	1.80	0.63
1:C:387:VAL:O	1:C:391:ILE:HG12	1.99	0.63
1:C:375:ILE:HG12	1:C:464:LEU:HD13	1.80	0.63
1:D:366:HIS:HE1	1:D:368:GLU:OE1	1.81	0.62
1:C:196:GLN:OE1	1:C:445:THR:N	2.31	0.62
1:A:185:CYS:HB2	1:E:363:TYR:CE2	2.33	0.62
1:E:68:LEU:HD22	1:E:203:THR:HG22	1.80	0.62
1:D:440:PRO:HG2	1:D:441:LEU:CD1	2.30	0.62
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.82	0.62
1:A:92:ASN:O	1:A:96:GLN:HG2	2.00	0.62
1:E:387:VAL:HG12	1:E:391:ILE:HD12	1.80	0.62
1:C:49:TYR:O	1:C:64:LYS:HE2	1.99	0.62
1:B:92:ASN:O	1:B:96:GLN:HG2	1.99	0.62
1:E:92:ASN:O	1:E:96:GLN:HG2	2.00	0.62
1:E:366:HIS:HE1	1:E:368:GLU:OE1	1.82	0.62
1:C:461:GLN:HE22	1:D:21:VAL:N	1.92	0.61
1:C:156:LEU:HG	1:C:334:VAL:HB	1.82	0.61
1:D:49:TYR:O	1:D:64:LYS:HE2	2.00	0.61
1:A:216:ASN:OD1	1:A:218:SER:HB2	2.01	0.61
1:B:68:LEU:HD22	1:B:203:THR:HG22	1.82	0.61
1:A:52:ILE:HB	1:A:62:VAL:HB	1.80	0.61
1:D:161:CYS:SG	1:D:244:ASP:HB3	2.40	0.61
1:A:68:LEU:HD22	1:A:203:THR:HG22	1.82	0.61
1:A:66:SER:H	1:A:69:GLN:NE2	1.98	0.61
1:C:366:HIS:HE1	1:C:368:GLU:OE1	1.84	0.61
1:C:68:LEU:HD22	1:C:203:THR:HG22	1.82	0.60
1:D:175:CYS:HB3	1:D:177:GLN:OE1	2.00	0.60
1:C:363:TYR:CD2	1:D:185:CYS:HB2	2.36	0.60
1:B:237:MET:SD	1:B:246:LEU:HD23	2.41	0.60
1:E:344:LEU:HD23	1:E:344:LEU:N	2.15	0.60
1:A:112:PRO:HB3	1:B:231:TYR:CD1	2.36	0.60
1:A:54:LYS:HG2	1:A:56:ASN:OD1	2.02	0.60
1:A:403:ASN:C	1:A:403:ASN:HD22	2.05	0.60
1:A:161:CYS:SG	1:A:244:ASP:HB3	2.41	0.60
1:A:49:TYR:O	1:A:64:LYS:HE2	2.02	0.60
1:D:240:GLU:HG2	1:D:243:GLY:H	1.66	0.60
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.84	0.59
1:B:461:GLN:HE22	1:C:21:VAL:N	1.88	0.59
1:D:68:LEU:HD13	1:D:151:TYR:HD1	1.67	0.59
1:C:112:PRO:HB3	1:D:231:TYR:CD1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:TYR:O	1:E:64:LYS:HE2	2.03	0.59
1:B:126:LEU:HB3	1:B:262:ASN:HB3	1.85	0.59
1:C:240:GLU:HG2	1:C:243:GLY:H	1.68	0.58
1:A:363:TYR:CE2	1:B:185:CYS:HB2	2.38	0.58
1:B:66:SER:H	1:B:69:GLN:NE2	1.99	0.58
1:A:293:PRO:HD3	1:E:117:ILE:HG21	1.85	0.58
1:D:387:VAL:HG12	1:D:391:ILE:HD12	1.84	0.58
1:C:403:ASN:HD22	1:C:403:ASN:C	2.07	0.58
1:C:92:ASN:O	1:C:96:GLN:HG2	2.04	0.58
1:E:156:LEU:HA	1:E:250:LEU:O	2.02	0.58
1:B:49:TYR:O	1:B:64:LYS:HE2	2.04	0.58
1:A:375:ILE:HG12	1:A:464:LEU:HD13	1.85	0.58
1:D:97:ARG:HG3	1:D:383:LEU:HD11	1.86	0.58
1:E:66:SER:H	1:E:69:GLN:NE2	2.00	0.58
1:B:175:CYS:HB3	1:B:177:GLN:OE1	2.03	0.58
1:C:78:PRO:HD3	1:C:452:LYS:HA	1.85	0.58
1:C:273:ASP:HA	1:C:276:TYR:CE2	2.39	0.57
1:C:246:LEU:O	1:C:246:LEU:HD12	2.04	0.57
1:B:181:GLN:HB2	1:B:184:ASP:OD1	2.04	0.57
1:D:120:HIS:HA	1:D:222:LEU:HD22	1.86	0.57
1:C:324:CYS:HB3	1:C:328:GLN:O	2.04	0.57
1:A:237:MET:SD	1:A:246:LEU:HD23	2.44	0.57
1:E:443:LYS:CA	1:E:443:LYS:HE2	2.32	0.57
1:C:441:LEU:HB3	1:C:444:TYR:HD1	1.70	0.57
1:B:216:ASN:OD1	1:B:218:SER:HB2	2.04	0.57
1:A:363:TYR:CD2	1:B:185:CYS:HB2	2.40	0.57
1:A:240:GLU:HG2	1:A:243:GLY:H	1.70	0.57
1:D:117:ILE:HG21	1:E:293:PRO:HD3	1.87	0.57
1:B:156:LEU:HG	1:B:334:VAL:HB	1.87	0.57
1:B:344:LEU:HD23	1:B:344:LEU:N	2.20	0.57
1:C:68:LEU:O	1:C:201:VAL:HG23	2.05	0.57
1:A:246:LEU:HD12	1:A:246:LEU:O	2.05	0.57
1:B:112:PRO:HB3	1:C:231:TYR:CD1	2.39	0.57
1:E:126:LEU:HB3	1:E:262:ASN:HB3	1.86	0.57
1:D:441:LEU:HB3	1:D:444:TYR:HD1	1.70	0.57
1:E:381:ILE:HD12	1:E:381:ILE:N	2.20	0.56
1:B:363:TYR:CE2	1:C:185:CYS:HB2	2.40	0.56
1:A:185:CYS:SG	1:E:365:ARG:NH1	2.79	0.56
1:E:161:CYS:SG	1:E:244:ASP:HB3	2.45	0.56
1:B:353:THR:O	1:D:278:LYS:HB2	2.06	0.56
1:D:55:PRO:HG2	1:D:56:ASN:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:LYS:HE2	1:D:443:LYS:CA	2.29	0.56
1:B:246:LEU:O	1:B:246:LEU:HD12	2.06	0.56
1:C:348:ILE:HG22	1:C:359:ASN:OD1	2.06	0.56
1:A:75:ILE:HB	1:A:329:LEU:HB3	1.87	0.56
1:B:278:LYS:HB2	1:E:353:THR:O	2.05	0.56
1:C:440:PRO:HG2	1:C:441:LEU:CD1	2.36	0.56
1:A:185:CYS:HB2	1:E:363:TYR:CD2	2.41	0.56
1:E:52:ILE:HB	1:E:62:VAL:HB	1.86	0.56
1:A:269:GLU:CD	1:E:52:ILE:HG12	2.26	0.56
1:D:52:ILE:HB	1:D:62:VAL:HB	1.86	0.56
1:E:273:ASP:HA	1:E:276:TYR:CE2	2.40	0.56
1:C:341:ASN:HD22	1:C:366:HIS:HB2	1.70	0.55
1:A:356:LYS:HB3	1:A:358:THR:HG23	1.87	0.55
1:D:156:LEU:HG	1:D:334:VAL:HB	1.89	0.55
1:C:54:LYS:HB3	1:C:57:ASN:CB	2.26	0.55
1:A:324:CYS:HB3	1:A:328:GLN:O	2.07	0.55
1:D:324:CYS:HB3	1:D:328:GLN:O	2.07	0.55
1:E:30:ARG:HB3	1:E:377:GLN:NE2	2.21	0.55
1:C:54:LYS:HG3	1:C:55:PRO:HD2	1.88	0.55
1:C:75:ILE:HB	1:C:329:LEU:HB3	1.88	0.55
1:E:216:ASN:OD1	1:E:218:SER:HB2	2.06	0.55
1:E:440:PRO:HG2	1:E:441:LEU:CD1	2.37	0.55
1:E:75:ILE:HB	1:E:329:LEU:HB3	1.89	0.55
1:A:231:TYR:CD1	1:E:112:PRO:HB3	2.41	0.55
1:E:441:LEU:HB3	1:E:444:TYR:HD1	1.70	0.55
1:E:240:GLU:HG2	1:E:243:GLY:H	1.72	0.55
1:D:273:ASP:HA	1:D:276:TYR:CE2	2.41	0.55
1:D:396:SER:O	1:D:400:GLU:HG3	2.07	0.55
1:D:92:ASN:O	1:D:96:GLN:HG2	2.06	0.55
1:D:54:LYS:HB3	1:D:57:ASN:HB2	1.89	0.55
1:D:348:ILE:HG22	1:D:359:ASN:OD1	2.07	0.55
1:E:54:LYS:HB2	1:E:57:ASN:HB3	1.90	0.55
1:C:276:TYR:HE1	1:C:278:LYS:HE3	1.72	0.54
1:A:117:ILE:HG21	1:B:293:PRO:HD3	1.88	0.54
1:B:395:ASN:HD22	1:B:395:ASN:C	2.09	0.54
1:B:324:CYS:HB3	1:B:328:GLN:O	2.07	0.54
1:D:166:GLY:HA3	1:D:195:ILE:HD11	1.88	0.54
1:A:57:ASN:OD1	1:A:59:LYS:HB3	2.07	0.54
1:D:381:ILE:N	1:D:381:ILE:HD12	2.22	0.54
1:D:68:LEU:O	1:D:201:VAL:HG23	2.07	0.54
1:B:96:GLN:HB3	1:B:382:THR:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HD13	1:B:151:TYR:HD1	1.72	0.54
1:E:54:LYS:CB	1:E:57:ASN:HB3	2.37	0.54
1:B:384:THR:OG1	1:B:387:VAL:HG23	2.06	0.54
1:E:156:LEU:HG	1:E:334:VAL:HB	1.89	0.54
1:B:150:ASP:O	1:B:296:SER:HA	2.07	0.54
1:B:366:HIS:HE1	1:B:368:GLU:OE1	1.89	0.54
1:B:54:LYS:HG3	1:B:55:PRO:HD2	1.90	0.54
1:B:440:PRO:HG2	1:B:441:LEU:CD1	2.37	0.54
1:D:112:PRO:HB3	1:E:231:TYR:CD1	2.42	0.54
1:A:440:PRO:HG2	1:A:441:LEU:CD1	2.38	0.54
1:B:161:CYS:SG	1:B:244:ASP:HB3	2.48	0.54
1:A:441:LEU:HB3	1:A:444:TYR:HD1	1.72	0.54
1:E:324:CYS:HB3	1:E:328:GLN:O	2.09	0.54
1:E:396:SER:O	1:E:400:GLU:HG3	2.08	0.54
1:B:260:LEU:N	1:B:260:LEU:HD12	2.23	0.54
1:D:344:LEU:HD23	1:D:344:LEU:N	2.23	0.54
1:B:68:LEU:O	1:B:201:VAL:HG23	2.08	0.53
1:D:46:GLY:HA3	1:D:65:VAL:HG23	1.89	0.53
1:A:68:LEU:O	1:A:201:VAL:HG23	2.07	0.53
1:D:120:HIS:ND1	1:D:121:PRO:HD2	2.23	0.53
1:E:116:GLY:O	1:E:117:ILE:HB	2.08	0.53
1:A:395:ASN:HD22	1:A:395:ASN:C	2.12	0.53
1:A:156:LEU:HG	1:A:334:VAL:HB	1.90	0.53
1:D:216:ASN:OD1	1:D:218:SER:HB2	2.09	0.53
1:E:68:LEU:HD13	1:E:151:TYR:HD1	1.73	0.53
1:A:120:HIS:ND1	1:A:121:PRO:HD2	2.23	0.53
1:C:55:PRO:HG2	1:C:56:ASN:H	1.74	0.53
1:D:156:LEU:HA	1:D:250:LEU:O	2.09	0.53
1:B:240:GLU:HG2	1:B:243:GLY:H	1.73	0.52
1:B:193:THR:HG21	1:B:230:LYS:HD2	1.90	0.52
1:A:344:LEU:HD12	1:B:186:PRO:HG2	1.91	0.52
1:C:24:THR:HG23	1:C:320:ASN:HA	1.91	0.52
1:A:260:LEU:HD12	1:A:260:LEU:N	2.24	0.52
1:E:401:ASP:O	1:E:402:TRP:O	2.27	0.52
1:D:164:PRO:HG2	1:D:195:ILE:HB	1.90	0.52
1:A:273:ASP:HA	1:A:276:TYR:CE2	2.44	0.52
1:C:97:ARG:HH21	1:C:403:ASN:CB	2.04	0.52
1:C:120:HIS:ND1	1:C:121:PRO:HD2	2.23	0.52
1:D:97:ARG:CG	1:D:383:LEU:HD11	2.40	0.52
1:C:161:CYS:SG	1:C:244:ASP:HB3	2.49	0.52
1:C:150:ASP:O	1:C:296:SER:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ILE:HB	1:D:329:LEU:HB3	1.92	0.52
1:E:246:LEU:O	1:E:246:LEU:HD12	2.10	0.52
1:B:348:ILE:HG22	1:B:359:ASN:OD1	2.08	0.52
1:B:471:GLN:OE1	1:B:472:LEU:HD23	2.08	0.52
1:E:395:ASN:C	1:E:395:ASN:HD22	2.12	0.52
1:B:74:ARG:HD2	1:B:76:HIS:CE1	2.44	0.52
1:E:126:LEU:HG	1:E:127:ASP:OD2	2.10	0.52
1:B:75:ILE:HB	1:B:329:LEU:HB3	1.90	0.52
1:A:156:LEU:HA	1:A:250:LEU:O	2.10	0.52
1:E:151:TYR:CG	1:E:203:THR:HB	2.45	0.52
1:E:74:ARG:HD2	1:E:76:HIS:CE1	2.45	0.52
1:A:193:THR:HG21	1:A:230:LYS:HD2	1.91	0.52
1:E:150:ASP:O	1:E:296:SER:HA	2.10	0.51
1:D:260:LEU:HD12	1:D:260:LEU:N	2.26	0.51
1:B:441:LEU:HB3	1:B:444:TYR:HD1	1.75	0.51
1:A:91:TYR:HD1	1:A:96:GLN:HG3	1.76	0.51
1:D:237:MET:SD	1:D:246:LEU:HD23	2.50	0.51
1:C:91:TYR:HD1	1:C:96:GLN:HG3	1.74	0.51
1:A:387:VAL:O	1:A:391:ILE:HD13	2.10	0.51
1:C:216:ASN:OD1	1:C:218:SER:HB2	2.11	0.51
1:D:193:THR:HG21	1:D:230:LYS:HD2	1.93	0.51
1:B:55:PRO:HG2	1:B:56:ASN:H	1.76	0.51
1:A:269:GLU:OE1	1:E:365:ARG:NH2	2.44	0.51
1:D:395:ASN:HD22	1:D:395:ASN:C	2.12	0.51
1:B:151:TYR:CG	1:B:203:THR:HB	2.45	0.51
1:B:443:LYS:HE2	1:B:443:LYS:CA	2.32	0.51
1:B:106:GLU:HG2	1:B:310:PRO:HA	1.93	0.51
1:D:96:GLN:HB3	1:D:382:THR:HA	1.93	0.51
1:D:403:ASN:C	1:D:403:ASN:HD22	2.13	0.51
1:C:445:THR:CG2	1:C:446:PHE:N	2.73	0.51
1:E:402:TRP:O	1:E:403:ASN:C	2.45	0.51
1:A:66:SER:H	1:A:69:GLN:HE21	1.59	0.51
1:E:65:VAL:HA	1:E:69:GLN:NE2	2.26	0.51
1:C:181:GLN:HB2	1:C:184:ASP:OD1	2.11	0.51
1:C:395:ASN:C	1:C:395:ASN:HD22	2.13	0.51
1:E:441:LEU:N	1:E:441:LEU:HD12	2.26	0.51
1:A:151:TYR:CG	1:A:203:THR:HB	2.46	0.51
1:C:151:TYR:CG	1:C:203:THR:HB	2.46	0.51
1:E:252:ARG:HD2	1:E:306:ILE:HD11	1.93	0.51
1:C:106:GLU:HG2	1:C:310:PRO:HA	1.94	0.50
1:D:150:ASP:O	1:D:296:SER:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLN:HB3	1:C:382:THR:HA	1.93	0.50
1:B:273:ASP:HA	1:B:276:TYR:CE2	2.46	0.50
1:E:380:LYS:C	1:E:381:ILE:HD12	2.31	0.50
1:B:120:HIS:HA	1:B:222:LEU:HD22	1.93	0.50
1:B:24:THR:HG23	1:B:320:ASN:HA	1.93	0.50
1:B:30:ARG:HB3	1:B:377:GLN:NE2	2.26	0.50
1:B:91:TYR:HD1	1:B:96:GLN:HG3	1.76	0.50
1:B:395:ASN:ND2	1:B:395:ASN:C	2.64	0.50
1:C:193:THR:HG21	1:C:230:LYS:HD2	1.94	0.50
1:D:30:ARG:HB3	1:D:377:GLN:NE2	2.27	0.50
1:A:55:PRO:HG2	1:A:56:ASN:H	1.76	0.50
1:A:401:ASP:O	1:A:402:TRP:O	2.29	0.50
1:B:403:ASN:C	1:B:403:ASN:HD22	2.15	0.50
1:E:55:PRO:HG2	1:E:56:ASN:H	1.77	0.50
1:A:222:LEU:O	1:A:225:CYS:HB3	2.12	0.50
1:E:164:PRO:HG2	1:E:195:ILE:HB	1.93	0.50
1:E:193:THR:HG21	1:E:230:LYS:HD2	1.94	0.50
1:B:341:ASN:HD22	1:B:366:HIS:HB2	1.77	0.50
1:C:74:ARG:HD2	1:C:76:HIS:CE1	2.47	0.50
1:B:381:ILE:HD12	1:B:381:ILE:N	2.26	0.49
1:D:66:SER:H	1:D:69:GLN:HE21	1.60	0.49
1:C:30:ARG:HB3	1:C:377:GLN:NE2	2.26	0.49
1:A:74:ARG:HD2	1:A:76:HIS:CE1	2.48	0.49
1:E:120:HIS:HA	1:E:222:LEU:HD22	1.93	0.49
1:D:151:TYR:CG	1:D:203:THR:HB	2.46	0.49
1:B:363:TYR:CD2	1:C:185:CYS:HB2	2.47	0.49
1:C:237:MET:SD	1:C:246:LEU:HD23	2.52	0.49
1:C:116:GLY:O	1:C:117:ILE:HB	2.13	0.49
1:A:186:PRO:HG2	1:E:344:LEU:HD12	1.94	0.49
1:D:91:TYR:HD1	1:D:96:GLN:HG3	1.77	0.49
1:C:120:HIS:HA	1:C:222:LEU:HD22	1.95	0.49
1:A:365:ARG:NH2	1:B:269:GLU:OE1	2.45	0.49
1:E:267:VAL:HG11	1:E:270:ASN:OD1	2.12	0.49
1:A:380:LYS:C	1:A:381:ILE:HD13	2.33	0.49
1:C:384:THR:OG1	1:C:387:VAL:HG23	2.12	0.49
1:E:74:ARG:HG2	1:E:330:PHE:CE2	2.48	0.49
1:A:120:HIS:HA	1:A:222:LEU:HD22	1.95	0.49
1:C:97:ARG:HG3	1:C:383:LEU:HD11	1.95	0.49
1:A:324:CYS:SG	1:A:329:LEU:HD23	2.53	0.49
1:C:214:GLN:OE1	1:C:219:GLU:HB2	2.13	0.49
1:B:99:VAL:HG23	1:B:381:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:CYS:SG	1:B:329:LEU:HD23	2.53	0.49
1:E:246:LEU:HD12	1:E:246:LEU:C	2.33	0.48
1:A:344:LEU:HD23	1:A:344:LEU:N	2.28	0.48
1:A:68:LEU:HD13	1:A:151:TYR:HD1	1.78	0.48
1:C:65:VAL:HA	1:C:69:GLN:NE2	2.28	0.48
1:E:68:LEU:O	1:E:201:VAL:HG23	2.13	0.48
1:E:96:GLN:HB3	1:E:382:THR:HA	1.94	0.48
1:A:65:VAL:HA	1:A:69:GLN:NE2	2.27	0.48
1:B:344:LEU:HD12	1:C:186:PRO:HG2	1.95	0.48
1:E:237:MET:O	1:E:240:GLU:HB3	2.14	0.48
1:D:341:ASN:HD22	1:D:366:HIS:HB2	1.77	0.48
1:C:69:GLN:NE2	1:C:71:ARG:NH2	2.62	0.48
1:D:65:VAL:HA	1:D:69:GLN:NE2	2.28	0.48
1:E:356:LYS:C	1:E:358:THR:H	2.17	0.48
1:B:54:LYS:HB3	1:B:57:ASN:CB	2.32	0.48
1:A:441:LEU:N	1:A:441:LEU:HD12	2.29	0.48
1:B:246:LEU:C	1:B:246:LEU:HD12	2.34	0.48
1:A:116:GLY:O	1:A:117:ILE:HB	2.13	0.48
1:A:176:THR:C	1:A:177:GLN:HG3	2.35	0.48
1:C:156:LEU:HA	1:C:250:LEU:O	2.14	0.48
1:E:237:MET:SD	1:E:246:LEU:HD23	2.53	0.48
1:E:125:LYS:O	1:E:125:LYS:HD3	2.14	0.48
1:A:54:LYS:HG3	1:A:55:PRO:HD2	1.96	0.48
1:C:225:CYS:SG	1:C:226:THR:HG23	2.54	0.48
1:C:65:VAL:HA	1:C:69:GLN:HE22	1.79	0.48
1:C:260:LEU:HD12	1:C:260:LEU:N	2.29	0.48
1:C:164:PRO:HG2	1:C:195:ILE:HB	1.96	0.47
1:A:24:THR:HG23	1:A:320:ASN:HA	1.96	0.47
1:E:120:HIS:ND1	1:E:121:PRO:HD2	2.28	0.47
1:A:96:GLN:HB3	1:A:382:THR:HA	1.95	0.47
1:D:279:GLY:HA3	1:D:283:THR:O	2.14	0.47
1:B:380:LYS:C	1:B:381:ILE:HD12	2.35	0.47
1:D:384:THR:OG1	1:D:387:VAL:HG23	2.15	0.47
1:A:106:GLU:OE2	1:A:467:LYS:NZ	2.46	0.47
1:A:395:ASN:ND2	1:A:395:ASN:C	2.68	0.47
1:A:366:HIS:CE1	1:A:368:GLU:OE1	2.57	0.47
1:B:341:ASN:ND2	1:B:366:HIS:CD2	2.82	0.47
1:A:150:ASP:O	1:A:296:SER:HA	2.14	0.47
1:D:297:GLY:O	1:D:298:SER:O	2.32	0.47
1:D:68:LEU:CD1	1:D:151:TYR:HD1	2.27	0.47
1:E:91:TYR:HD1	1:E:96:GLN:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:GLY:O	1:E:298:SER:O	2.33	0.47
1:A:181:GLN:HB2	1:A:184:ASP:OD1	2.15	0.47
1:B:99:VAL:HG23	1:B:381:ILE:HD13	1.97	0.47
1:D:24:THR:HG23	1:D:320:ASN:HA	1.96	0.47
1:C:344:LEU:HD12	1:D:186:PRO:HG2	1.96	0.47
1:B:297:GLY:O	1:B:298:SER:O	2.33	0.47
1:D:181:GLN:HB2	1:D:184:ASP:OD1	2.14	0.47
1:D:68:LEU:HD13	1:D:151:TYR:CD1	2.47	0.47
1:A:171:LYS:HG3	1:A:186:PRO:HB2	1.97	0.47
1:C:237:MET:O	1:C:240:GLU:HB3	2.14	0.47
1:A:106:GLU:HG2	1:A:310:PRO:HA	1.97	0.47
1:C:171:LYS:HG3	1:C:186:PRO:HB2	1.97	0.47
1:E:171:LYS:HG3	1:E:186:PRO:HB2	1.96	0.47
1:A:30:ARG:HB3	1:A:377:GLN:NE2	2.30	0.47
1:D:106:GLU:HG2	1:D:310:PRO:HA	1.97	0.47
1:A:201:VAL:O	1:A:203:THR:HG23	2.15	0.47
1:B:156:LEU:HA	1:B:250:LEU:O	2.15	0.46
1:C:344:LEU:HD23	1:C:344:LEU:N	2.29	0.46
1:D:74:ARG:HG2	1:D:330:PHE:CZ	2.50	0.46
1:D:380:LYS:C	1:D:381:ILE:HD12	2.35	0.46
1:D:441:LEU:HD12	1:D:441:LEU:N	2.30	0.46
1:A:341:ASN:HD22	1:A:366:HIS:HB2	1.81	0.46
1:C:441:LEU:HD12	1:C:441:LEU:N	2.30	0.46
1:C:68:LEU:HD13	1:C:151:TYR:HD1	1.79	0.46
1:A:279:GLY:HA3	1:A:283:THR:O	2.15	0.46
1:A:65:VAL:HA	1:A:69:GLN:HE22	1.81	0.46
1:C:126:LEU:HG	1:C:127:ASP:OD2	2.15	0.46
1:E:471:GLN:OE1	1:E:472:LEU:HD23	2.14	0.46
1:E:106:GLU:HG2	1:E:310:PRO:HA	1.97	0.46
1:D:344:LEU:HD12	1:E:186:PRO:HG2	1.97	0.46
1:B:119:GLY:O	1:B:222:LEU:HD22	2.16	0.46
1:E:341:ASN:HD22	1:E:366:HIS:HB2	1.79	0.46
1:B:201:VAL:O	1:B:203:THR:HG23	2.16	0.46
1:C:201:VAL:O	1:C:203:THR:HG23	2.16	0.46
1:B:96:GLN:HE21	1:B:96:GLN:HB3	1.56	0.46
1:C:246:LEU:C	1:C:246:LEU:HD12	2.36	0.46
1:A:164:PRO:HG2	1:A:195:ILE:HB	1.97	0.46
1:D:120:HIS:HA	1:D:222:LEU:CD2	2.46	0.46
1:A:341:ASN:ND2	1:A:366:HIS:CD2	2.83	0.46
1:D:65:VAL:HA	1:D:69:GLN:HE22	1.81	0.46
1:B:333:VAL:HG12	1:B:334:VAL:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ILE:H	1:D:33:ILE:HG12	1.63	0.46
1:B:52:ILE:HG12	1:C:269:GLU:CD	2.37	0.45
1:B:106:GLU:HB2	1:B:464:LEU:HG	1.98	0.45
1:C:355:TYR:HE2	1:C:357:ASN:ND2	2.14	0.45
1:E:70:TYR:OH	1:E:232:PRO:HD3	2.16	0.45
1:B:125:LYS:O	1:B:125:LYS:HD3	2.16	0.45
1:D:341:ASN:ND2	1:D:366:HIS:CD2	2.84	0.45
1:B:69:GLN:NE2	1:B:71:ARG:NH2	2.64	0.45
1:D:262:ASN:HA	1:D:262:ASN:HD22	1.51	0.45
1:E:96:GLN:HB3	1:E:96:GLN:HE21	1.62	0.45
1:E:395:ASN:C	1:E:395:ASN:ND2	2.70	0.45
1:C:74:ARG:HG2	1:C:330:PHE:CZ	2.52	0.45
1:C:106:GLU:HB2	1:C:464:LEU:HG	1.99	0.45
1:A:97:ARG:HG3	1:A:383:LEU:HD11	1.98	0.45
1:B:239:SER:O	1:B:240:GLU:C	2.55	0.45
1:E:99:VAL:HG23	1:E:381:ILE:CD1	2.47	0.45
1:D:99:VAL:HG23	1:D:381:ILE:CD1	2.46	0.45
1:E:106:GLU:HB2	1:E:464:LEU:HG	1.98	0.45
1:E:384:THR:OG1	1:E:387:VAL:HG23	2.16	0.45
1:E:24:THR:HG23	1:E:320:ASN:HA	1.98	0.45
1:A:239:SER:O	1:A:240:GLU:C	2.55	0.45
1:A:246:LEU:HD12	1:A:246:LEU:C	2.37	0.45
1:D:395:ASN:ND2	1:D:395:ASN:C	2.70	0.45
1:D:74:ARG:HG2	1:D:330:PHE:CE2	2.52	0.45
1:C:342:MET:HB2	1:D:208:MET:SD	2.57	0.45
1:A:138:ASN:HD22	1:A:138:ASN:HA	1.63	0.45
1:B:300:VAL:O	1:C:254:GLN:HA	2.17	0.45
1:C:395:ASN:C	1:C:395:ASN:ND2	2.70	0.45
1:C:395:ASN:O	1:C:398:ILE:HG12	2.17	0.45
1:D:363:TYR:CE2	1:E:185:CYS:HB2	2.51	0.45
1:B:365:ARG:NH2	1:C:269:GLU:OE1	2.48	0.45
1:C:324:CYS:SG	1:C:329:LEU:HD23	2.57	0.45
1:E:239:SER:O	1:E:240:GLU:C	2.55	0.45
1:C:74:ARG:HG2	1:C:330:PHE:CE2	2.52	0.45
1:D:171:LYS:HG3	1:D:186:PRO:HB2	1.99	0.45
1:C:97:ARG:CG	1:C:383:LEU:HD11	2.48	0.44
1:E:341:ASN:ND2	1:E:366:HIS:CD2	2.86	0.44
1:A:74:ARG:HG2	1:A:330:PHE:CZ	2.52	0.44
1:A:396:SER:O	1:A:400:GLU:HG3	2.17	0.44
1:B:117:ILE:CG2	1:C:293:PRO:HD3	2.46	0.44
1:E:151:TYR:CD2	1:E:203:THR:HB	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:HG	1:B:127:ASP:OD2	2.17	0.44
1:B:65:VAL:HA	1:B:69:GLN:NE2	2.33	0.44
1:D:116:GLY:O	1:D:117:ILE:HB	2.17	0.44
1:E:290:ASN:HA	1:E:290:ASN:HD22	1.60	0.44
1:B:237:MET:O	1:B:240:GLU:HB3	2.17	0.44
1:A:237:MET:O	1:A:240:GLU:HB3	2.17	0.44
1:A:355:TYR:HE2	1:A:357:ASN:ND2	2.14	0.44
1:E:260:LEU:HD12	1:E:260:LEU:N	2.32	0.44
1:D:358:THR:HA	1:E:266:THR:CG2	2.47	0.44
1:D:96:GLN:HB3	1:D:96:GLN:HE21	1.59	0.44
1:C:222:LEU:O	1:C:225:CYS:HB3	2.17	0.44
1:D:246:LEU:O	1:D:246:LEU:HD12	2.17	0.44
1:E:74:ARG:HG2	1:E:330:PHE:CZ	2.52	0.44
1:E:356:LYS:C	1:E:358:THR:N	2.69	0.44
1:A:74:ARG:HG2	1:A:330:PHE:CE2	2.53	0.44
1:A:125:LYS:O	1:A:125:LYS:HD3	2.18	0.44
1:D:365:ARG:NH2	1:E:269:GLU:OE1	2.51	0.44
1:A:126:LEU:HG	1:A:127:ASP:OD2	2.17	0.44
1:B:342:MET:HB2	1:C:208:MET:SD	2.57	0.44
1:A:274:ASP:O	1:E:217:LYS:HE2	2.18	0.44
1:E:136:ALA:O	1:E:137:ALA:O	2.36	0.44
1:C:92:ASN:OD1	1:C:94:ASP:HB2	2.18	0.44
1:C:276:TYR:CE1	1:C:278:LYS:HE3	2.53	0.44
1:E:54:LYS:HB3	1:E:57:ASN:CB	2.47	0.44
1:D:363:TYR:CD2	1:E:185:CYS:HB2	2.53	0.44
1:A:297:GLY:O	1:A:298:SER:O	2.36	0.44
1:D:471:GLN:OE1	1:D:472:LEU:HD23	2.18	0.44
1:D:461:GLN:HE22	1:E:21:VAL:N	1.90	0.43
1:B:391:ILE:HD12	1:B:391:ILE:N	2.33	0.43
1:A:96:GLN:HE21	1:A:96:GLN:HB3	1.57	0.43
1:E:222:LEU:O	1:E:225:CYS:HB3	2.18	0.43
1:E:324:CYS:SG	1:E:329:LEU:HD23	2.58	0.43
1:A:235:ILE:H	1:A:235:ILE:HD12	1.83	0.43
1:B:138:ASN:HD22	1:B:138:ASN:HA	1.66	0.43
1:B:116:GLY:O	1:B:117:ILE:HB	2.18	0.43
1:C:220:VAL:HB	1:C:224:ILE:HD11	1.99	0.43
1:C:70:TYR:OH	1:C:232:PRO:HD3	2.18	0.43
1:A:208:MET:SD	1:E:342:MET:HB2	2.57	0.43
1:D:92:ASN:OD1	1:D:94:ASP:HB2	2.18	0.43
1:B:222:LEU:O	1:B:225:CYS:HB3	2.17	0.43
1:C:197:ASP:CB	1:C:446:PHE:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:PRO:HG2	1:B:195:ILE:HB	1.99	0.43
1:A:103:VAL:O	1:A:103:VAL:HG12	2.18	0.43
1:A:342:MET:HB2	1:B:208:MET:SD	2.59	0.43
1:A:70:TYR:OH	1:A:232:PRO:HD3	2.18	0.43
1:D:99:VAL:HG23	1:D:381:ILE:HD13	2.00	0.43
1:C:239:SER:O	1:C:240:GLU:C	2.56	0.43
1:D:60:ILE:HD12	1:D:60:ILE:H	1.84	0.43
1:B:110:GLY:O	1:C:167:GLU:OE2	2.37	0.43
1:D:355:TYR:HE2	1:D:357:ASN:ND2	2.16	0.43
1:D:239:SER:O	1:D:240:GLU:C	2.57	0.43
1:C:66:SER:H	1:C:69:GLN:HE21	1.62	0.43
1:D:237:MET:O	1:D:240:GLU:HB3	2.18	0.43
1:D:138:ASN:HA	1:D:138:ASN:HD22	1.60	0.43
1:E:99:VAL:HG23	1:E:381:ILE:HD13	2.00	0.43
1:E:92:ASN:HA	1:E:93:PRO:HD2	1.91	0.43
1:D:136:ALA:O	1:D:137:ALA:O	2.37	0.43
1:E:39:THR:HG23	1:E:372:LEU:HB2	2.01	0.43
1:D:92:ASN:HA	1:D:93:PRO:HD2	1.92	0.42
1:A:22:VAL:HG22	1:A:390:TYR:CE1	2.54	0.42
1:D:106:GLU:HB2	1:D:464:LEU:HG	2.00	0.42
1:E:65:VAL:HA	1:E:69:GLN:HE22	1.82	0.42
1:A:54:LYS:CG	1:A:56:ASN:OD1	2.66	0.42
1:E:120:HIS:HB2	1:E:221:PRO:HA	2.00	0.42
1:B:441:LEU:N	1:B:441:LEU:HD12	2.34	0.42
1:C:341:ASN:ND2	1:C:366:HIS:CD2	2.88	0.42
1:B:171:LYS:HG3	1:B:186:PRO:HB2	2.01	0.42
1:A:22:VAL:HB	1:A:26:GLU:HG3	2.00	0.42
1:E:60:ILE:H	1:E:60:ILE:HD12	1.84	0.42
1:E:46:GLY:HA3	1:E:65:VAL:HG23	2.01	0.42
1:C:157:CYS:O	1:C:249:TYR:HA	2.20	0.42
1:B:103:VAL:HG12	1:B:103:VAL:O	2.20	0.42
1:D:151:TYR:CD2	1:D:203:THR:HB	2.54	0.42
1:C:117:ILE:CG2	1:D:293:PRO:HD3	2.48	0.42
1:D:351:SER:HB2	1:D:352:GLU:H	1.70	0.42
1:D:201:VAL:O	1:D:203:THR:HG23	2.20	0.42
1:D:124:ASN:OD1	1:D:264:ALA:HB3	2.20	0.42
1:A:234:TYR:O	1:A:238:VAL:HG23	2.20	0.42
1:C:401:ASP:O	1:C:402:TRP:O	2.38	0.42
1:C:443:LYS:HB2	1:C:443:LYS:HE3	1.53	0.42
1:B:68:LEU:CD1	1:B:151:TYR:HD1	2.33	0.42
1:B:151:TYR:CD2	1:B:203:THR:HB	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:THR:CG2	1:B:320:ASN:HA	2.50	0.42
1:B:357:ASN:ND2	1:C:264:ALA:HB1	2.35	0.42
1:E:366:HIS:CE1	1:E:368:GLU:OE1	2.69	0.42
1:B:355:TYR:HE2	1:B:357:ASN:ND2	2.18	0.42
1:B:97:ARG:HG3	1:B:383:LEU:HD11	2.01	0.41
1:B:39:THR:HB	1:B:42:LEU:HD21	2.01	0.41
1:E:119:GLY:O	1:E:222:LEU:HD22	2.20	0.41
1:B:365:ARG:NH1	1:C:185:CYS:SG	2.94	0.41
1:A:266:THR:HG23	1:E:358:THR:HA	2.02	0.41
1:D:74:ARG:HD2	1:D:76:HIS:CE1	2.55	0.41
1:C:232:PRO:HB2	1:C:234:TYR:CE1	2.55	0.41
1:A:107:VAL:O	1:A:307:PHE:HB3	2.20	0.41
1:C:341:ASN:ND2	1:C:366:HIS:HB2	2.35	0.41
1:B:351:SER:HB2	1:B:352:GLU:H	1.66	0.41
1:B:66:SER:H	1:B:69:GLN:HE21	1.66	0.41
1:B:333:VAL:CG1	1:B:334:VAL:N	2.83	0.41
1:D:395:ASN:O	1:D:398:ILE:HG13	2.20	0.41
1:D:119:GLY:O	1:D:222:LEU:HD22	2.21	0.41
1:A:199:ASP:CG	1:A:230:LYS:HE2	2.41	0.41
1:B:65:VAL:HA	1:B:69:GLN:HE22	1.86	0.41
1:E:66:SER:H	1:E:69:GLN:HE21	1.64	0.41
1:B:341:ASN:ND2	1:B:366:HIS:HD2	2.18	0.41
1:E:193:THR:CG2	1:E:230:LYS:HD2	2.51	0.41
1:A:267:VAL:HG11	1:A:270:ASN:HA	2.03	0.41
1:A:39:THR:HG23	1:A:372:LEU:HB2	2.03	0.41
1:B:72:VAL:HG22	1:B:332:THR:HG23	2.02	0.41
1:B:197:ASP:CB	1:B:446:PHE:HA	2.50	0.41
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.85	0.41
1:B:120:HIS:HA	1:B:222:LEU:CD2	2.50	0.41
1:B:120:HIS:ND1	1:B:121:PRO:HD2	2.36	0.41
1:C:445:THR:C	1:C:446:PHE:CG	2.94	0.41
1:A:293:PRO:HD3	1:E:117:ILE:CG2	2.51	0.41
1:B:232:PRO:HB2	1:B:234:TYR:CE1	2.56	0.41
1:B:358:THR:HA	1:C:266:THR:CG2	2.51	0.41
1:E:374:PHE:HB2	1:E:376:PHE:CE1	2.56	0.41
1:A:120:HIS:HB2	1:A:221:PRO:HA	2.04	0.41
1:D:106:GLU:OE2	1:D:467:LYS:NZ	2.48	0.41
1:E:92:ASN:OD1	1:E:94:ASP:HB2	2.21	0.41
1:B:193:THR:CG2	1:B:230:LYS:HD2	2.49	0.41
1:D:72:VAL:HG22	1:D:332:THR:HG23	2.03	0.41
1:D:197:ASP:CB	1:D:446:PHE:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:VAL:O	1:E:103:VAL:HG12	2.20	0.41
1:C:471:GLN:OE1	1:C:472:LEU:HD23	2.21	0.41
1:B:21:VAL:HG12	1:B:22:VAL:N	2.36	0.40
1:A:214:GLN:OE1	1:A:219:GLU:HB2	2.21	0.40
1:E:262:ASN:HA	1:E:262:ASN:HD22	1.53	0.40
1:D:324:CYS:SG	1:D:329:LEU:HD23	2.61	0.40
1:B:247:PHE:CZ	1:B:322:GLY:HA2	2.56	0.40
1:D:232:PRO:HB2	1:D:234:TYR:CE1	2.56	0.40
1:D:401:ASP:O	1:D:402:TRP:O	2.39	0.40
1:E:204:GLY:HA2	1:E:255:MET:HE2	2.02	0.40
1:D:22:VAL:HG22	1:D:390:TYR:CE1	2.56	0.40
1:C:103:VAL:HG12	1:C:103:VAL:O	2.20	0.40
1:D:121:PRO:HD3	1:D:222:LEU:CD2	2.37	0.40
1:A:106:GLU:HB2	1:A:464:LEU:HG	2.03	0.40
1:D:472:LEU:O	1:D:474:LEU:N	2.55	0.40
1:B:42:LEU:HB3	1:B:447:TRP:CZ2	2.56	0.40
1:C:297:GLY:O	1:C:298:SER:O	2.39	0.40
1:C:72:VAL:HG22	1:C:332:THR:HG23	2.04	0.40
1:B:124:ASN:OD1	1:B:264:ALA:HB3	2.22	0.40
1:D:374:PHE:CD1	1:D:374:PHE:N	2.90	0.40
1:A:178:VAL:HG23	1:A:178:VAL:H	1.61	0.40
1:B:33:ILE:HG12	1:B:33:ILE:H	1.70	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	417/455 (92%)	378 (91%)	29 (7%)	10 (2%)	7 47
1	B	417/455 (92%)	377 (90%)	30 (7%)	10 (2%)	7 47
1	C	417/455 (92%)	376 (90%)	33 (8%)	8 (2%)	10 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	417/455 (92%)	377 (90%)	30 (7%)	10 (2%)	7	47
1	E	417/455 (92%)	378 (91%)	31 (7%)	8 (2%)	10	52
All	All	2085/2275 (92%)	1886 (90%)	153 (7%)	46 (2%)	13	49

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ALA
1	A	298	SER
1	A	402	TRP
1	B	137	ALA
1	B	298	SER
1	C	137	ALA
1	C	298	SER
1	C	402	TRP
1	D	137	ALA
1	D	298	SER
1	D	402	TRP
1	E	137	ALA
1	E	298	SER
1	E	402	TRP
1	A	117	ILE
1	A	126	LEU
1	B	126	LEU
1	B	402	TRP
1	B	473	GLY
1	C	117	ILE
1	C	126	LEU
1	C	473	GLY
1	D	126	LEU
1	D	473	GLY
1	E	117	ILE
1	E	126	LEU
1	E	473	GLY
1	A	41	ARG
1	A	473	GLY
1	B	41	ARG
1	C	41	ARG
1	D	41	ARG
1	E	41	ARG
1	A	177	GLN

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Mol	Chain	Res	Type
1	B	177	GLN
1	D	117	ILE
1	A	142	ASP
1	B	117	ILE
1	B	142	ASP
1	C	177	GLN
1	E	177	GLN
1	D	142	ASP
1	D	177	GLN
1	A	178	VAL
1	D	178	VAL
1	B	178	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	368/396 (93%)	334 (91%)	34 (9%)	11	43
1	B	368/396 (93%)	335 (91%)	33 (9%)	12	44
1	C	368/396 (93%)	329 (89%)	39 (11%)	8	36
1	D	368/396 (93%)	334 (91%)	34 (9%)	11	43
1	E	368/396 (93%)	330 (90%)	38 (10%)	9	37
All	All	1840/1980 (93%)	1662 (90%)	178 (10%)	15	40

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	33	ILE
1	A	60	ILE
1	A	66	SER
1	A	68	LEU
1	A	74	ARG
1	A	96	GLN

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Mol	Chain	Res	Type
1	A	106	GLU
1	A	127	ASP
1	A	138	ASN
1	A	193	THR
1	A	213	LEU
1	A	246	LEU
1	A	247	PHE
1	A	251	ARG
1	A	262	ASN
1	A	286	LEU
1	A	301	THR
1	A	315	ARG
1	A	317	GLN
1	A	344	LEU
1	A	348	ILE
1	A	352	GLU
1	A	358	THR
1	A	386	ASP
1	A	395	ASN
1	A	403	ASN
1	A	438	GLU
1	A	441	LEU
1	A	446	PHE
1	A	453	GLU
1	A	464	LEU
1	A	472	LEU
1	A	474	LEU
1	B	32	ASN
1	B	33	ILE
1	B	54	LYS
1	B	60	ILE
1	B	66	SER
1	B	74	ARG
1	B	91	TYR
1	B	96	GLN
1	B	106	GLU
1	B	127	ASP
1	B	138	ASN
1	B	193	THR
1	B	213	LEU
1	B	246	LEU
1	B	247	PHE

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Mol	Chain	Res	Type
1	B	251	ARG
1	B	262	ASN
1	B	286	LEU
1	B	301	THR
1	B	315	ARG
1	B	317	GLN
1	B	344	LEU
1	B	352	GLU
1	B	386	ASP
1	B	395	ASN
1	B	403	ASN
1	B	438	GLU
1	B	441	LEU
1	B	446	PHE
1	B	453	GLU
1	B	464	LEU
1	B	472	LEU
1	B	474	LEU
1	C	32	ASN
1	C	33	ILE
1	C	54	LYS
1	C	60	ILE
1	C	66	SER
1	C	74	ARG
1	C	91	TYR
1	C	96	GLN
1	C	106	GLU
1	C	127	ASP
1	C	138	ASN
1	C	178	VAL
1	C	193	THR
1	C	213	LEU
1	C	225	CYS
1	C	246	LEU
1	C	247	PHE
1	C	251	ARG
1	C	262	ASN
1	C	278	LYS
1	C	286	LEU
1	C	301	THR
1	C	315	ARG
1	C	317	GLN

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Mol	Chain	Res	Type
1	C	344	LEU
1	C	348	ILE
1	C	351	SER
1	C	352	GLU
1	C	386	ASP
1	C	395	ASN
1	C	403	ASN
1	C	438	GLU
1	C	441	LEU
1	C	443	LYS
1	C	446	PHE
1	C	453	GLU
1	C	464	LEU
1	C	472	LEU
1	C	474	LEU
1	D	32	ASN
1	D	33	ILE
1	D	60	ILE
1	D	74	ARG
1	D	91	TYR
1	D	95	THR
1	D	96	GLN
1	D	106	GLU
1	D	127	ASP
1	D	135	TYR
1	D	138	ASN
1	D	193	THR
1	D	213	LEU
1	D	246	LEU
1	D	247	PHE
1	D	251	ARG
1	D	262	ASN
1	D	270	ASN
1	D	286	LEU
1	D	301	THR
1	D	315	ARG
1	D	317	GLN
1	D	342	MET
1	D	344	LEU
1	D	352	GLU
1	D	395	ASN
1	D	403	ASN

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Mol	Chain	Res	Type
1	D	438	GLU
1	D	441	LEU
1	D	446	PHE
1	D	453	GLU
1	D	464	LEU
1	D	472	LEU
1	D	474	LEU
1	E	32	ASN
1	E	33	ILE
1	E	54	LYS
1	E	60	ILE
1	E	66	SER
1	E	68	LEU
1	E	74	ARG
1	E	82	LYS
1	E	91	TYR
1	E	96	GLN
1	E	106	GLU
1	E	117	ILE
1	E	127	ASP
1	E	138	ASN
1	E	193	THR
1	E	213	LEU
1	E	246	LEU
1	E	247	PHE
1	E	251	ARG
1	E	262	ASN
1	E	286	LEU
1	E	301	THR
1	E	306	ILE
1	E	315	ARG
1	E	317	GLN
1	E	344	LEU
1	E	345	CYS
1	E	352	GLU
1	E	386	ASP
1	E	395	ASN
1	E	403	ASN
1	E	438	GLU
1	E	441	LEU
1	E	446	PHE
1	E	453	GLU

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Mol	Chain	Res	Type
1	E	464	LEU
1	E	472	LEU
1	E	474	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	69	GLN
1	A	138	ASN
1	A	153	GLN
1	A	192	ASN
1	A	259	HIS
1	A	262	ASN
1	A	290	ASN
1	A	341	ASN
1	A	366	HIS
1	A	395	ASN
1	A	403	ASN
1	A	461	GLN
1	B	32	ASN
1	B	69	GLN
1	B	96	GLN
1	B	138	ASN
1	B	153	GLN
1	B	259	HIS
1	B	262	ASN
1	B	290	ASN
1	B	341	ASN
1	B	366	HIS
1	B	395	ASN
1	B	403	ASN
1	B	461	GLN
1	C	32	ASN
1	C	69	GLN
1	C	138	ASN
1	C	153	GLN
1	C	262	ASN
1	C	290	ASN
1	C	341	ASN
1	C	366	HIS
1	C	395	ASN

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Mol	Chain	Res	Type
1	C	403	ASN
1	C	461	GLN
1	D	32	ASN
1	D	69	GLN
1	D	96	GLN
1	D	138	ASN
1	D	153	GLN
1	D	192	ASN
1	D	262	ASN
1	D	270	ASN
1	D	290	ASN
1	D	341	ASN
1	D	366	HIS
1	D	395	ASN
1	D	403	ASN
1	D	461	GLN
1	E	32	ASN
1	E	69	GLN
1	E	138	ASN
1	E	153	GLN
1	E	262	ASN
1	E	290	ASN
1	E	341	ASN
1	E	366	HIS
1	E	395	ASN
1	E	403	ASN
1	E	461	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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.