



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 21, 2017 – 05:04 PM EDT

PDB ID : 3JCB
EMDB ID: : EMD-6542
Title : Structure of Simian Immunodeficiency Virus Envelope Spikes bound with CD4
and Monoclonal Antibody 36D5
Authors : Hu, G.; Liu, J.; Roux, K.; Taylor, K.A.
Deposited on : unknown
Resolution : unknown (reported)
Based on PDB ID : 4NCO

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

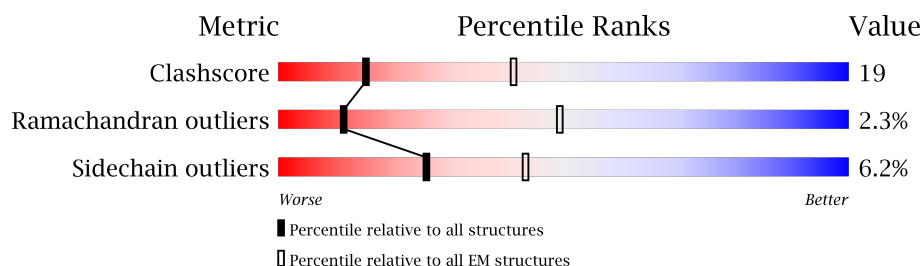
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	448	
1	E	448	
1	I	448	
2	B	207	
3	C	232	
4	D	175	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13909 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	420	Total	C	N	O	S	0	0
			3096	1937	544	590	25		
1	E	420	Total	C	N	O	S	0	0
			3096	1937	544	590	25		
1	I	420	Total	C	N	O	S	0	0
			3096	1937	544	590	25		

- Molecule 2 is a protein called Antibody 36D5 light chain.

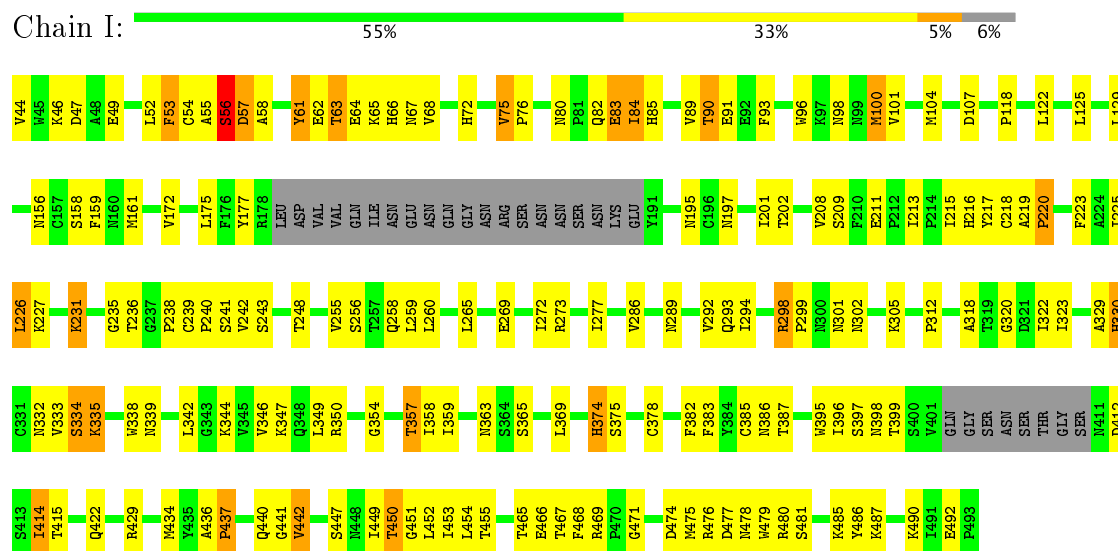
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	202	Total	C	N	O	S	0	0
			1530	964	255	307	4		

- Molecule 3 is a protein called Antibody 36D5 heavy chain.

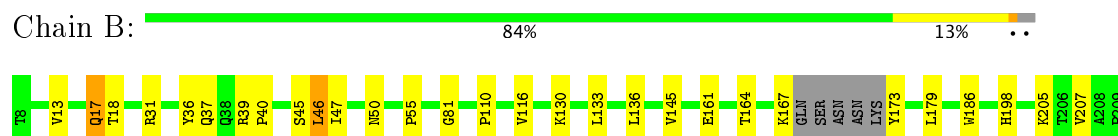
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	226	Total	C	N	O	S	0	0
			1728	1100	293	330	5		

- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

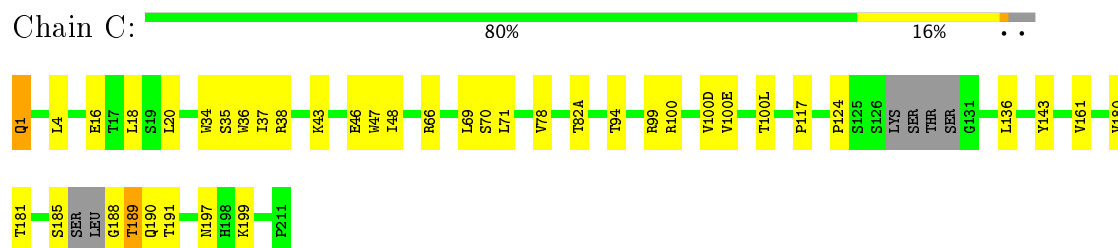
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1363	851	239	269	4		



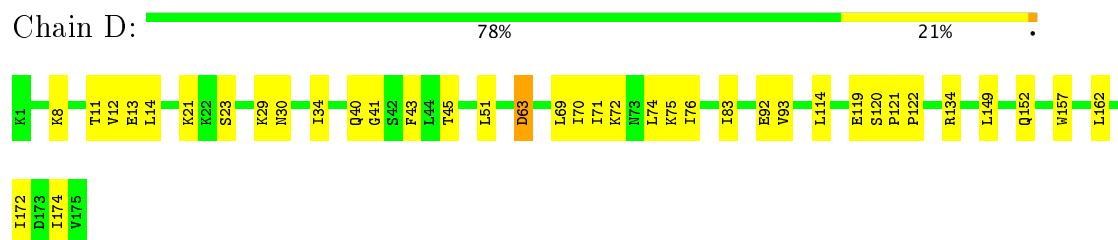
- Molecule 2: Antibody 36D5 light chain



- Molecule 3: Antibody 36D5 heavy chain



- Molecule 4: T-cell surface glycoprotein CD4



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	1181	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	31000	Depositor
Image detector	TVIPS TEMCAM-F415 (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	0.33	0/3161	0.71	4/4306 (0.1%)
1	E	0.34	0/3161	0.71	4/4306 (0.1%)
1	I	0.34	0/3161	0.71	3/4306 (0.1%)
2	B	0.28	0/1571	0.54	1/2151 (0.0%)
3	C	0.31	0/1774	0.57	0/2421
4	D	0.26	0/1382	0.53	0/1863
All	All	0.32	0/14210	0.66	12/19353 (0.1%)

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	3
1	E	0	3
1	I	0	3
2	B	0	1
All	All	0	10

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	LYS	N-CA-C	6.19	127.72	111.00
1	I	335	LYS	N-CA-C	6.19	127.71	111.00
1	E	335	LYS	N-CA-C	6.18	127.70	111.00
1	E	450	THR	C-N-CA	-5.98	109.74	122.30
1	A	450	THR	C-N-CA	-5.97	109.76	122.30
1	I	450	THR	C-N-CA	-5.96	109.79	122.30
1	A	334	SER	C-N-CA	5.52	135.50	121.70
1	E	334	SER	C-N-CA	5.52	135.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	334	SER	C-N-CA	5.50	135.44	121.70
2	B	46	LEU	CA-CB-CG	5.31	127.52	115.30
1	E	259	LEU	C-N-CA	-5.02	109.16	121.70
1	A	259	LEU	C-N-CA	-5.01	109.17	121.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	THR	Peptide
1	A	56	SER	Peptide
1	A	80	ASN	Peptide
2	B	110	PRO	Peptide
1	E	236	THR	Peptide
1	E	56	SER	Peptide
1	E	80	ASN	Peptide
1	I	236	THR	Peptide
1	I	56	SER	Peptide
1	I	80	ASN	Peptide

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	3096	0	2836	159	0
1	E	3096	0	2836	127	0
1	I	3096	0	2835	150	0
2	B	1530	0	1472	19	0
3	C	1728	0	1699	37	0
4	D	1363	0	1386	61	0
All	All	13909	0	13064	501	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 (501) 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)
4:D:21:LYS:CE	1:I:62:GLU:HG3	1.41	1.49
1:A:472:GLY:O	4:D:40:GLN:HG3	1.16	1.27
4:D:21:LYS:HE3	1:I:62:GLU:CG	1.63	1.26
1:A:325:ASP:O	3:C:100(E):VAL:HG23	1.15	1.25
1:A:474:ASP:OD1	4:D:41:GLY:HA3	1.04	1.22
1:A:325:ASP:O	3:C:100(E):VAL:CG2	1.85	1.21
1:A:472:GLY:O	4:D:40:GLN:CG	1.91	1.18
1:A:474:ASP:OD1	4:D:41:GLY:CA	1.92	1.18
4:D:21:LYS:CE	1:I:62:GLU:CG	2.17	1.18
4:D:21:LYS:HD2	1:I:62:GLU:HB2	1.17	1.12
4:D:21:LYS:NZ	1:I:62:GLU:HG3	1.63	1.11
1:A:293:GLN:HB2	1:A:334:SER:HB3	1.33	1.10
1:I:293:GLN:HB2	1:I:334:SER:HB3	1.33	1.05
1:E:293:GLN:HB2	1:E:334:SER:HB3	1.33	1.04
4:D:21:LYS:CE	1:I:61:TYR:HB3	1.86	1.04
4:D:21:LYS:NZ	1:I:62:GLU:CG	2.18	1.01
4:D:21:LYS:CD	1:I:62:GLU:HB2	1.97	0.93
4:D:21:LYS:HE3	1:I:62:GLU:HG3	0.93	0.92
4:D:76:ILE:H	4:D:76:ILE:HD12	1.35	0.92
4:D:21:LYS:CD	1:I:61:TYR:HB3	1.99	0.92
4:D:21:LYS:HD3	1:I:61:TYR:HB3	1.53	0.88
1:I:91:GLU:HA	1:I:239:CYS:O	1.74	0.87
1:A:474:ASP:CG	4:D:41:GLY:HA3	1.94	0.87
1:A:91:GLU:HA	1:A:239:CYS:O	1.74	0.87
1:A:326:ILE:HA	3:C:100(E):VAL:HB	1.56	0.87
1:E:91:GLU:HA	1:E:239:CYS:O	1.74	0.87
1:E:358:ILE:HB	1:E:465:THR:HG22	1.57	0.86
4:D:21:LYS:CE	1:I:62:GLU:CB	2.53	0.85
4:D:21:LYS:HD2	1:I:62:GLU:CB	2.05	0.85
1:I:358:ILE:HB	1:I:465:THR:HG22	1.58	0.84
1:A:324:GLY:O	3:C:100(E):VAL:HG21	1.76	0.84
1:A:358:ILE:HB	1:A:465:THR:HG22	1.58	0.84
1:A:260:LEU:HB2	1:A:450:THR:O	1.78	0.83
1:I:260:LEU:HB2	1:I:450:THR:O	1.78	0.82
1:E:260:LEU:HB2	1:E:450:THR:O	1.78	0.82
3:C:38:ARG:N	3:C:46:GLU:O	2.12	0.80
1:A:269:GLU:HA	1:A:289:ASN:HD22	1.48	0.78
1:I:269:GLU:HA	1:I:289:ASN:HD22	1.48	0.78
3:C:38:ARG:O	3:C:46:GLU:N	2.15	0.78
1:E:335:LYS:HD3	1:E:414:ILE:HD11	1.67	0.76
1:E:269:GLU:HA	1:E:289:ASN:HD22	1.48	0.76
1:I:335:LYS:HD3	1:I:414:ILE:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ALA:HB3	1:E:216:HIS:HB2	1.68	0.76
1:A:335:LYS:HD3	1:A:414:ILE:HD11	1.67	0.75
3:C:99:ARG:HG2	3:C:100(L):THR:HG22	1.68	0.75
1:I:55:ALA:HB3	1:I:216:HIS:HB2	1.68	0.75
1:A:472:GLY:O	4:D:40:GLN:CB	2.34	0.75
1:E:436:ALA:HB3	1:E:437:PRO:HD3	1.70	0.74
1:I:101:VAL:HG13	1:I:479:TRP:HB2	1.69	0.74
1:E:101:VAL:HG13	1:E:479:TRP:HB2	1.69	0.74
1:A:474:ASP:CG	4:D:41:GLY:CA	2.52	0.74
1:I:436:ALA:HB3	1:I:437:PRO:HD3	1.70	0.73
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.68	0.73
1:A:101:VAL:HG13	1:A:479:TRP:HB2	1.69	0.73
1:A:325:ASP:C	3:C:100(E):VAL:CG2	2.57	0.73
1:A:325:ASP:C	3:C:100(E):VAL:HG23	2.06	0.73
1:A:436:ALA:HB3	1:A:437:PRO:HD3	1.70	0.72
1:A:199:SER:HA	1:I:312:PRO:HB3	1.73	0.71
1:A:325:ASP:O	3:C:100(E):VAL:CB	2.40	0.69
1:E:227:LYS:HE3	1:E:485:LYS:HD2	1.75	0.69
4:D:29:LYS:HB2	4:D:83:ILE:HD11	1.74	0.69
4:D:21:LYS:CE	1:I:61:TYR:CB	2.68	0.69
1:I:227:LYS:HE3	1:I:485:LYS:HD2	1.75	0.69
4:D:21:LYS:HE3	1:I:62:GLU:CD	2.13	0.69
1:A:227:LYS:HE3	1:A:485:LYS:HD2	1.75	0.68
3:C:37:ILE:HG23	3:C:47:TRP:HA	1.76	0.68
1:A:330:HIS:CD2	3:C:100(D):VAL:CG2	2.77	0.68
1:I:294:ILE:HG23	1:I:447:SER:HB2	1.76	0.67
1:I:477:ASP:OD1	1:I:480:ARG:NH1	2.27	0.67
1:A:294:ILE:HG23	1:A:447:SER:HB2	1.76	0.67
1:E:477:ASP:OD1	1:E:480:ARG:NH1	2.27	0.67
2:B:39:ARG:HG3	2:B:40:PRO:HD2	1.77	0.67
3:C:38:ARG:O	3:C:46:GLU:O	2.12	0.67
4:D:21:LYS:HE2	1:I:61:TYR:HB3	1.72	0.67
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.27	0.67
1:A:472:GLY:C	4:D:40:GLN:HE21	1.98	0.66
4:D:21:LYS:HE2	1:I:61:TYR:CG	2.31	0.66
1:A:350:ARG:NH2	1:A:397:SER:O	2.30	0.65
1:E:294:ILE:HG23	1:E:447:SER:HB2	1.76	0.65
1:E:350:ARG:NH2	1:E:397:SER:O	2.29	0.65
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.79	0.64
3:C:35:SER:HB3	3:C:47:TRP:HE1	1.62	0.64
4:D:51:LEU:HD23	4:D:71:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:VAL:HG21	1:E:480:ARG:HG2	1.79	0.64
1:I:350:ARG:NH2	1:I:397:SER:O	2.30	0.64
4:D:21:LYS:CD	1:I:62:GLU:CB	2.67	0.64
1:I:68:VAL:O	1:I:72:HIS:ND1	2.31	0.64
1:E:68:VAL:O	1:E:72:HIS:ND1	2.31	0.63
1:A:68:VAL:O	1:A:72:HIS:ND1	2.31	0.63
2:B:37:GLN:N	2:B:45:SER:O	2.31	0.63
1:I:101:VAL:HG21	1:I:480:ARG:HG2	1.79	0.63
1:I:359:ILE:HD12	1:I:468:PHE:HE1	1.63	0.63
1:E:91:GLU:O	1:E:238:PRO:HA	1.99	0.63
1:A:359:ILE:HD12	1:A:468:PHE:HE1	1.63	0.63
1:E:359:ILE:HD12	1:E:468:PHE:HE1	1.63	0.62
4:D:21:LYS:HE2	1:I:61:TYR:CB	2.27	0.62
1:E:100:MET:N	1:E:100:MET:SD	2.73	0.62
1:A:91:GLU:O	1:A:238:PRO:HA	1.99	0.62
1:I:91:GLU:O	1:I:238:PRO:HA	1.99	0.62
1:A:363:ASN:O	1:A:469:ARG:NH1	2.33	0.62
1:E:226:LEU:HD11	1:E:487:LYS:HD3	1.82	0.61
1:I:100:MET:SD	1:I:100:MET:N	2.73	0.61
1:I:83:GLU:HG3	1:I:84:ILE:H	1.65	0.61
1:E:363:ASN:O	1:E:469:ARG:NH1	2.33	0.61
1:A:83:GLU:HG3	1:A:84:ILE:H	1.65	0.61
1:I:226:LEU:HD11	1:I:487:LYS:HD3	1.82	0.61
1:I:363:ASN:O	1:I:469:ARG:NH1	2.33	0.61
4:D:83:ILE:HG22	4:D:92:GLU:HG2	1.83	0.61
1:E:83:GLU:HG3	1:E:84:ILE:H	1.65	0.60
1:I:358:ILE:HG13	1:I:397:SER:H	1.66	0.60
1:A:100:MET:N	1:A:100:MET:SD	2.73	0.60
1:A:226:LEU:HD11	1:A:487:LYS:HD3	1.82	0.60
1:A:226:LEU:HD11	1:A:487:LYS:HB3	1.83	0.60
1:I:177:TYR:HE2	1:I:422:GLN:HE21	1.49	0.60
1:E:358:ILE:HG13	1:E:397:SER:H	1.66	0.60
1:E:226:LEU:HD11	1:E:487:LYS:HB3	1.84	0.60
1:I:226:LEU:HD11	1:I:487:LYS:HB3	1.83	0.60
1:A:177:TYR:HE2	1:A:422:GLN:HE21	1.49	0.59
4:D:76:ILE:HD12	4:D:76:ILE:N	2.12	0.59
1:E:258:GLN:O	1:E:452:LEU:HA	2.03	0.59
1:A:258:GLN:O	1:A:452:LEU:HA	2.03	0.59
2:B:37:GLN:O	2:B:45:SER:O	2.20	0.59
3:C:37:ILE:HG13	3:C:47:TRP:HD1	1.67	0.59
1:A:358:ILE:HG13	1:A:397:SER:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ARG:HA	1:A:479:TRP:CD1	2.38	0.59
1:I:258:GLN:O	1:I:452:LEU:HA	2.03	0.59
1:A:52:LEU:HB3	1:A:217:TYR:HD2	1.68	0.59
1:I:256:SER:HB2	1:I:374:HIS:HE1	1.68	0.59
1:A:256:SER:HB2	1:A:374:HIS:HE1	1.68	0.58
2:B:50:ASN:OD1	3:C:100:ARG:NH2	2.36	0.58
1:A:226:LEU:CD1	1:A:487:LYS:HB3	2.33	0.58
1:A:371:VAL:HG11	4:D:45:THR:HG22	1.85	0.58
1:E:177:TYR:HE2	1:E:422:GLN:HE21	1.49	0.58
1:I:52:LEU:HB3	1:I:217:TYR:HD2	1.68	0.58
1:E:52:LEU:HB3	1:E:217:TYR:HD2	1.68	0.58
1:I:476:ARG:HA	1:I:479:TRP:CD1	2.38	0.58
1:E:256:SER:HB2	1:E:374:HIS:HE1	1.69	0.58
1:I:226:LEU:CD1	1:I:487:LYS:HB3	2.33	0.58
1:I:259:LEU:HB3	1:I:449:ILE:HG23	1.85	0.58
1:A:259:LEU:HB3	1:A:449:ILE:HG23	1.85	0.58
1:E:476:ARG:HA	1:E:479:TRP:CD1	2.38	0.58
1:A:122:LEU:HA	1:A:201:ILE:HA	1.86	0.57
1:I:422:GLN:O	1:I:434:MET:HA	2.04	0.57
2:B:145:VAL:HG12	2:B:198:HIS:HB2	1.86	0.57
3:C:4:LEU:HD11	3:C:94:THR:HG23	1.85	0.57
1:I:98:ASN:HB3	1:I:100:MET:HG2	1.87	0.57
1:I:122:LEU:HA	1:I:201:ILE:HA	1.85	0.57
1:A:330:HIS:CD2	3:C:100(D):VAL:HG21	2.39	0.57
1:E:122:LEU:HA	1:E:201:ILE:HA	1.85	0.57
1:E:98:ASN:HB3	1:E:100:MET:HG2	1.87	0.57
1:A:98:ASN:HB3	1:A:100:MET:HG2	1.87	0.57
2:B:36:TYR:HA	2:B:46:LEU:HA	1.85	0.57
1:E:226:LEU:CD1	1:E:487:LYS:HB3	2.34	0.57
4:D:76:ILE:CD1	4:D:76:ILE:H	2.11	0.57
1:I:53:PHE:HB3	1:I:218:CYS:HB2	1.87	0.57
1:A:53:PHE:HB3	1:A:218:CYS:HB2	1.87	0.56
1:E:259:LEU:HB3	1:E:449:ILE:HG23	1.85	0.56
1:A:422:GLN:O	1:A:434:MET:HA	2.05	0.56
1:E:53:PHE:HB3	1:E:218:CYS:HB2	1.87	0.56
1:E:422:GLN:O	1:E:434:MET:HA	2.05	0.56
1:A:474:ASP:OD2	4:D:41:GLY:CA	2.53	0.56
1:E:347:LYS:O	1:E:350:ARG:HG2	2.06	0.56
1:E:82:GLN:O	1:E:84:ILE:HG13	2.06	0.56
1:A:347:LYS:O	1:A:350:ARG:HG2	2.06	0.55
3:C:37:ILE:HG13	3:C:47:TRP:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:VAL:HG22	3:C:180:VAL:HG12	1.88	0.55
1:I:82:GLN:O	1:I:84:ILE:HG13	2.06	0.55
1:E:217:TYR:O	1:E:248:THR:HG23	2.07	0.55
1:I:347:LYS:O	1:I:350:ARG:HG2	2.06	0.55
1:A:82:GLN:O	1:A:84:ILE:HG13	2.06	0.55
1:A:217:TYR:O	1:A:248:THR:HG23	2.07	0.55
3:C:37:ILE:HA	3:C:47:TRP:HA	1.89	0.55
1:E:93:PHE:CE1	1:E:226:LEU:HD13	2.42	0.55
1:I:217:TYR:O	1:I:248:THR:HG23	2.07	0.55
2:B:39:ARG:NH1	2:B:81:GLY:O	2.40	0.55
1:A:326:ILE:CA	3:C:100(E):VAL:HB	2.35	0.54
1:I:451:GLY:O	1:I:452:LEU:HD23	2.07	0.54
1:I:93:PHE:CE1	1:I:226:LEU:HD13	2.42	0.54
1:E:451:GLY:O	1:E:452:LEU:HD23	2.07	0.54
1:I:346:VAL:HG21	1:I:395:TRP:CD1	2.43	0.54
1:A:93:PHE:CE1	1:A:226:LEU:HD13	2.42	0.54
1:I:396:ILE:HG22	1:I:398:ASN:H	1.73	0.54
4:D:23:SER:HB3	4:D:63:ASP:HA	1.88	0.54
1:I:63:THR:OG1	1:I:64:GLU:N	2.40	0.54
1:E:346:VAL:HG21	1:E:395:TRP:CD1	2.43	0.54
3:C:34:TRP:CZ3	3:C:94:THR:HG22	2.43	0.54
1:E:344:LYS:HA	1:E:347:LYS:HE2	1.90	0.54
1:E:298:ARG:HG2	1:E:383:PHE:CZ	2.43	0.54
4:D:14:LEU:HB2	4:D:69:LEU:HB3	1.90	0.54
1:I:298:ARG:HG2	1:I:383:PHE:CZ	2.43	0.54
1:I:82:GLN:O	1:I:84:ILE:N	2.41	0.54
1:A:346:VAL:HG21	1:A:395:TRP:CD1	2.43	0.53
1:A:451:GLY:O	1:A:452:LEU:HD23	2.07	0.53
1:A:63:THR:OG1	1:A:64:GLU:N	2.40	0.53
4:D:74:LEU:HD13	4:D:75:LYS:N	2.22	0.53
1:A:396:ILE:HG22	1:A:398:ASN:H	1.73	0.53
1:E:66:HIS:HB3	1:E:213:ILE:HG12	1.90	0.53
1:E:82:GLN:O	1:E:84:ILE:N	2.42	0.53
1:A:66:HIS:HB3	1:A:213:ILE:HG12	1.90	0.53
1:I:66:HIS:HB3	1:I:213:ILE:HG12	1.90	0.53
1:E:396:ILE:HG22	1:E:398:ASN:H	1.73	0.53
2:B:37:GLN:HB2	2:B:47:ILE:HG12	1.91	0.53
1:I:344:LYS:HA	1:I:347:LYS:HE2	1.90	0.53
1:I:378:CYS:HB2	1:I:383:PHE:CE1	2.44	0.53
1:A:298:ARG:HG2	1:A:383:PHE:CZ	2.43	0.53
1:A:344:LYS:HA	1:A:347:LYS:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:O	1:A:216:HIS:ND1	2.42	0.53
1:A:305:LYS:O	1:A:318:ALA:N	2.42	0.53
1:A:82:GLN:O	1:A:84:ILE:N	2.41	0.53
1:E:305:LYS:O	1:E:318:ALA:N	2.42	0.53
1:E:378:CYS:HB2	1:E:383:PHE:CE1	2.44	0.53
1:A:64:GLU:HB2	1:A:209:SER:HB3	1.90	0.52
1:I:305:LYS:O	1:I:318:ALA:N	2.42	0.52
1:A:265:LEU:HD23	1:A:450:THR:HG23	1.91	0.52
1:I:55:ALA:O	1:I:216:HIS:ND1	2.42	0.52
1:I:265:LEU:HD23	1:I:450:THR:HG23	1.91	0.52
1:E:299:PRO:HA	1:E:442:VAL:HA	1.91	0.52
1:A:378:CYS:HB2	1:A:383:PHE:CE1	2.44	0.52
4:D:30:ASN:HD21	4:D:34:ILE:HB	1.75	0.52
1:I:299:PRO:HA	1:I:442:VAL:HA	1.91	0.52
1:A:159:PHE:HB2	1:A:172:VAL:HG23	1.92	0.52
1:E:64:GLU:HB2	1:E:209:SER:HB3	1.90	0.52
1:E:63:THR:OG1	1:E:64:GLU:N	2.40	0.52
1:I:64:GLU:HB2	1:I:209:SER:HB3	1.90	0.52
2:B:133:LEU:HD12	2:B:179:LEU:HD23	1.92	0.52
3:C:189:THR:OG1	3:C:190:GLN:N	2.42	0.52
1:E:265:LEU:HD23	1:E:450:THR:HG23	1.91	0.52
1:E:55:ALA:O	1:E:216:HIS:ND1	2.42	0.51
1:E:346:VAL:HA	1:E:349:LEU:HD12	1.92	0.51
1:A:299:PRO:HA	1:A:442:VAL:HA	1.91	0.51
1:I:346:VAL:HA	1:I:349:LEU:HD12	1.92	0.51
1:I:478:ASN:O	1:I:481:SER:OG	2.20	0.51
1:A:93:PHE:HE1	1:A:226:LEU:HD13	1.75	0.51
1:I:159:PHE:HB2	1:I:172:VAL:HG23	1.92	0.51
4:D:14:LEU:HD12	4:D:69:LEU:HD12	1.93	0.51
1:E:248:THR:HG22	1:E:486:TYR:CE1	2.46	0.51
1:A:64:GLU:HA	1:A:209:SER:N	2.26	0.51
3:C:185:SER:O	3:C:188:GLY:N	2.44	0.51
1:A:248:THR:HG22	1:A:486:TYR:CE1	2.46	0.51
1:E:64:GLU:HA	1:E:209:SER:N	2.26	0.51
1:I:248:THR:HG22	1:I:486:TYR:CE1	2.46	0.51
1:I:64:GLU:HA	1:I:209:SER:N	2.26	0.51
1:A:335:LYS:HG3	1:A:339:ASN:OD1	2.11	0.50
1:A:346:VAL:HA	1:A:349:LEU:HD12	1.92	0.50
1:I:335:LYS:HG3	1:I:339:ASN:OD1	2.11	0.50
1:I:158:SER:O	1:I:159:PHE:HD1	1.95	0.50
1:E:159:PHE:HB2	1:E:172:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:LYS:HG3	1:E:339:ASN:OD1	2.11	0.50
1:I:90:THR:HG22	1:I:91:GLU:H	1.76	0.50
1:A:158:SER:O	1:A:159:PHE:HD1	1.95	0.50
4:D:70:ILE:O	4:D:71:ILE:HD13	2.10	0.50
1:E:158:SER:O	1:E:159:PHE:HD1	1.95	0.50
1:E:93:PHE:HE1	1:E:226:LEU:HD13	1.75	0.50
1:I:474:ASP:HB3	1:I:476:ARG:HG2	1.94	0.50
1:A:478:ASN:O	1:A:481:SER:OG	2.20	0.50
1:A:46:LYS:HB3	1:A:490:LYS:HG3	1.94	0.50
4:D:8:LYS:HA	4:D:74:LEU:HD12	1.92	0.50
1:A:474:ASP:HB3	1:A:476:ARG:HG2	1.94	0.50
4:D:157:TRP:HB2	4:D:172:ILE:HG13	1.93	0.50
1:I:93:PHE:HE1	1:I:226:LEU:HD13	1.75	0.50
1:I:96:TRP:HZ2	1:I:273:ARG:HB3	1.77	0.50
1:A:226:LEU:HA	1:A:243:SER:O	2.12	0.50
1:E:474:ASP:HB3	1:E:476:ARG:HG2	1.94	0.50
1:I:129:LEU:HA	1:I:159:PHE:CE1	2.47	0.49
1:A:90:THR:HG22	1:A:91:GLU:H	1.76	0.49
1:I:46:LYS:HB3	1:I:490:LYS:HG3	1.94	0.49
1:E:46:LYS:HB3	1:E:490:LYS:HG3	1.94	0.49
1:I:286:VAL:HB	1:I:452:LEU:HB2	1.94	0.49
1:E:96:TRP:HZ2	1:E:273:ARG:HB3	1.76	0.49
1:E:90:THR:HG22	1:E:91:GLU:H	1.76	0.49
1:A:455:THR:HG23	1:A:471:GLY:HA3	1.95	0.49
1:A:371:VAL:CG2	4:D:43:PHE:HB3	2.43	0.49
1:E:129:LEU:HA	1:E:159:PHE:CE1	2.47	0.49
1:E:55:ALA:HB3	1:E:216:HIS:CB	2.42	0.49
1:A:129:LEU:HA	1:A:159:PHE:CE1	2.48	0.49
2:B:37:GLN:HB2	2:B:47:ILE:CG1	2.43	0.49
1:I:226:LEU:HA	1:I:243:SER:O	2.12	0.49
1:I:455:THR:HG23	1:I:471:GLY:HA3	1.95	0.49
1:E:226:LEU:HA	1:E:243:SER:O	2.12	0.48
1:E:286:VAL:HB	1:E:452:LEU:HB2	1.94	0.48
1:E:455:THR:HG23	1:E:471:GLY:HA3	1.95	0.48
1:E:129:LEU:HA	1:E:159:PHE:HE1	1.79	0.48
1:E:85:HIS:CE1	1:E:241:SER:HA	2.49	0.48
1:E:65:LYS:HG3	1:E:208:VAL:HB	1.96	0.48
1:I:129:LEU:HA	1:I:159:PHE:HE1	1.79	0.48
1:A:65:LYS:HG3	1:A:208:VAL:HB	1.96	0.48
1:A:96:TRP:HZ2	1:A:273:ARG:HB3	1.77	0.48
1:A:286:VAL:HB	1:A:452:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TYR:HB3	2:B:45:SER:O	2.14	0.47
4:D:21:LYS:HD3	1:I:61:TYR:CB	2.37	0.47
1:E:365:SER:HB2	1:E:469:ARG:HD3	1.96	0.47
1:I:375:SER:HA	1:I:383:PHE:O	2.14	0.47
1:I:65:LYS:HG3	1:I:208:VAL:HB	1.96	0.47
1:A:129:LEU:HA	1:A:159:PHE:HE1	1.79	0.47
1:A:473:GLY:HA3	4:D:40:GLN:HB3	1.96	0.47
1:E:375:SER:HA	1:E:383:PHE:O	2.14	0.47
1:E:49:GLU:HG3	1:E:223:PHE:HE2	1.79	0.47
4:D:157:TRP:CE2	4:D:174:ILE:HD12	2.49	0.47
1:E:161:MET:HE2	1:E:172:VAL:HG11	1.97	0.47
1:E:239:CYS:HA	1:E:240:PRO:HD3	1.46	0.47
1:A:129:LEU:HG	1:A:159:PHE:CZ	2.49	0.47
1:A:202:THR:HA	1:A:434:MET:HB2	1.96	0.47
1:I:64:GLU:OE2	1:I:211:GLU:N	2.48	0.47
1:I:85:HIS:CE1	1:I:241:SER:HA	2.49	0.47
1:A:365:SER:HB2	1:A:469:ARG:HD3	1.96	0.47
1:A:375:SER:HA	1:A:383:PHE:O	2.14	0.47
1:A:85:HIS:CE1	1:A:241:SER:HA	2.49	0.47
2:B:17:GLN:CD	2:B:18:THR:H	2.18	0.47
1:E:202:THR:HA	1:E:434:MET:HB2	1.96	0.47
1:E:64:GLU:OE2	1:E:211:GLU:N	2.48	0.47
1:I:175:LEU:HD21	1:I:320:GLY:HA3	1.97	0.47
1:I:49:GLU:HG3	1:I:223:PHE:HE2	1.79	0.47
1:A:259:LEU:HD13	1:A:449:ILE:HD13	1.97	0.47
1:A:75:VAL:HG22	1:A:76:PRO:HD2	1.97	0.47
1:E:175:LEU:HD21	1:E:320:GLY:HA3	1.97	0.47
1:E:64:GLU:HG2	1:E:67:ASN:H	1.80	0.47
1:E:75:VAL:HG22	1:E:76:PRO:HD2	1.97	0.47
4:D:114:LEU:HB2	4:D:149:LEU:HD11	1.96	0.47
1:E:85:HIS:CE1	1:E:242:VAL:H	2.34	0.47
1:E:272:ILE:HG22	1:E:286:VAL:HG13	1.98	0.46
1:A:49:GLU:HG3	1:A:223:PHE:HE2	1.79	0.46
1:A:64:GLU:HG2	1:A:67:ASN:H	1.80	0.46
1:I:129:LEU:HG	1:I:159:PHE:CZ	2.49	0.46
1:I:332:ASN:OD1	1:I:415:THR:HG23	2.16	0.46
1:I:202:THR:HA	1:I:434:MET:HB2	1.96	0.46
1:A:55:ALA:HB3	1:A:216:HIS:CB	2.42	0.46
3:C:36:TRP:HE1	3:C:78:VAL:HG12	1.80	0.46
1:E:85:HIS:ND1	1:E:242:VAL:O	2.37	0.46
1:I:272:ILE:HG22	1:I:286:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:57:ASP:OD1	1:I:58:ALA:N	2.49	0.46
1:A:85:HIS:CE1	1:A:242:VAL:H	2.34	0.46
1:A:333:VAL:HG13	1:A:414:ILE:HD12	1.97	0.46
1:A:354:GLY:O	1:A:357:THR:OG1	2.34	0.46
1:A:64:GLU:OE2	1:A:211:GLU:N	2.48	0.46
4:D:83:ILE:C	4:D:83:ILE:HD12	2.35	0.46
1:E:333:VAL:HG13	1:E:414:ILE:HD12	1.97	0.46
1:E:57:ASP:OD1	1:E:58:ALA:N	2.49	0.46
1:A:57:ASP:OD1	1:A:58:ALA:N	2.49	0.46
3:C:124:PRO:HG3	3:C:136:LEU:HG	1.97	0.46
1:E:354:GLY:O	1:E:357:THR:OG1	2.34	0.46
1:I:75:VAL:HG22	1:I:76:PRO:HD2	1.97	0.46
1:A:161:MET:HE2	1:A:172:VAL:HG11	1.98	0.46
1:I:298:ARG:HB3	1:I:329:ALA:HB1	1.98	0.46
1:A:332:ASN:OD1	1:A:415:THR:HG23	2.16	0.46
1:I:85:HIS:CE1	1:I:242:VAL:H	2.33	0.46
1:A:96:TRP:CH2	1:A:235:GLY:HA3	2.51	0.46
1:A:371:VAL:CG1	4:D:45:THR:HG22	2.46	0.46
1:E:129:LEU:HG	1:E:159:PHE:CZ	2.49	0.46
1:E:259:LEU:HD13	1:E:449:ILE:HD13	1.98	0.46
1:E:298:ARG:HB3	1:E:329:ALA:HB1	1.98	0.46
1:A:175:LEU:HD21	1:A:320:GLY:HA3	1.97	0.46
1:I:354:GLY:O	1:I:357:THR:OG1	2.34	0.45
1:I:55:ALA:HB3	1:I:216:HIS:CB	2.41	0.45
1:I:64:GLU:HG2	1:I:67:ASN:H	1.80	0.45
1:I:96:TRP:CH2	1:I:235:GLY:HA3	2.51	0.45
1:A:272:ILE:HG22	1:A:286:VAL:HG13	1.98	0.45
1:I:333:VAL:HG13	1:I:414:ILE:HD12	1.97	0.45
1:A:65:LYS:NZ	1:A:208:VAL:HG11	2.32	0.45
1:E:65:LYS:NZ	1:E:208:VAL:HG11	2.32	0.45
1:I:365:SER:HB2	1:I:469:ARG:HD3	1.96	0.45
1:I:65:LYS:NZ	1:I:208:VAL:HG11	2.32	0.45
3:C:47:TRP:O	3:C:48:ILE:HG13	2.16	0.45
1:A:474:ASP:OD1	4:D:40:GLN:O	2.35	0.45
1:E:96:TRP:CH2	1:E:235:GLY:HA3	2.51	0.45
1:I:259:LEU:HD13	1:I:449:ILE:HD13	1.97	0.45
1:A:472:GLY:CA	4:D:40:GLN:HE21	2.30	0.45
3:C:66:ARG:HD2	3:C:82(A):THR:O	2.17	0.45
1:E:332:ASN:OD1	1:E:415:THR:HG23	2.16	0.45
1:E:440:GLN:HB3	1:E:441:GLY:H	1.53	0.45
1:A:298:ARG:HB3	1:A:329:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:422:GLN:OE1	1:I:436:ALA:HA	2.17	0.45
1:E:478:ASN:O	1:E:481:SER:OG	2.20	0.44
2:B:116:VAL:HG23	2:B:205:LYS:HD2	2.00	0.44
2:B:37:GLN:O	2:B:45:SER:C	2.56	0.44
1:E:298:ARG:HG2	1:E:383:PHE:HZ	1.82	0.44
1:E:422:GLN:OE1	1:E:436:ALA:HA	2.17	0.44
1:E:260:LEU:HD21	1:E:481:SER:OG	2.18	0.44
1:I:259:LEU:HA	1:I:451:GLY:O	2.18	0.44
1:A:219:ALA:HB2	1:A:225:ILE:HG13	2.00	0.44
1:A:220:PRO:HG2	1:A:223:PHE:CD1	2.53	0.44
1:I:219:ALA:HB2	1:I:225:ILE:HG13	2.00	0.44
1:I:220:PRO:HG2	1:I:223:PHE:CD1	2.53	0.44
1:I:239:CYS:HA	1:I:240:PRO:HD3	1.46	0.44
1:A:298:ARG:HG3	1:A:298:ARG:H	1.58	0.44
1:A:259:LEU:HA	1:A:451:GLY:O	2.18	0.44
1:A:474:ASP:CG	4:D:41:GLY:N	2.70	0.44
1:E:219:ALA:HB2	1:E:225:ILE:HG13	2.00	0.44
1:A:260:LEU:HD21	1:A:481:SER:OG	2.18	0.44
1:A:369:LEU:HG	1:A:369:LEU:H	1.58	0.44
1:A:422:GLN:OE1	1:A:436:ALA:HA	2.17	0.44
1:A:239:CYS:HA	1:A:240:PRO:HD3	1.46	0.43
1:E:220:PRO:HG2	1:E:223:PHE:CD1	2.53	0.43
1:A:63:THR:O	1:A:208:VAL:HA	2.18	0.43
1:E:61:TYR:HB3	1:E:62:GLU:H	1.53	0.43
1:I:54:CYS:SG	1:I:215:ILE:HG23	2.58	0.43
1:I:298:ARG:HG2	1:I:383:PHE:HZ	1.82	0.43
1:I:255:VAL:HG13	1:I:475:MET:SD	2.58	0.43
1:A:255:VAL:HG13	1:A:475:MET:SD	2.58	0.43
1:A:85:HIS:ND1	1:A:242:VAL:O	2.36	0.43
1:E:93:PHE:HD2	1:E:239:CYS:HB3	1.84	0.43
1:A:436:ALA:CB	1:A:437:PRO:HD3	2.46	0.43
2:B:46:LEU:HD23	2:B:55:PRO:HG3	1.99	0.43
1:E:54:CYS:SG	1:E:215:ILE:HG23	2.58	0.43
1:I:260:LEU:HD21	1:I:481:SER:OG	2.18	0.43
2:B:167:LYS:HE3	2:B:173:TYR:CE1	2.52	0.43
2:B:186:TRP:HH2	2:B:207:VAL:HG22	1.83	0.43
1:E:259:LEU:HA	1:E:451:GLY:O	2.18	0.43
1:A:129:LEU:HG	1:A:159:PHE:HZ	1.84	0.43
1:A:416:LEU:HA	1:A:417:PRO:HD3	1.65	0.43
1:A:54:CYS:SG	1:A:215:ILE:HG23	2.58	0.43
1:E:255:VAL:HG13	1:E:475:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:453:ILE:O	1:I:454:LEU:HD23	2.19	0.43
1:A:453:ILE:O	1:A:454:LEU:HD23	2.19	0.43
1:E:63:THR:O	1:E:208:VAL:HA	2.19	0.43
1:E:330:HIS:CE1	1:E:415:THR:HG21	2.54	0.43
1:E:416:LEU:HA	1:E:417:PRO:HD3	1.65	0.43
3:C:38:ARG:O	3:C:46:GLU:C	2.57	0.43
1:E:369:LEU:H	1:E:369:LEU:HG	1.58	0.42
1:A:199:SER:CA	1:I:312:PRO:HB3	2.45	0.42
1:A:104:MET:HG3	1:A:217:TYR:OH	2.19	0.42
1:E:292:VAL:HB	1:E:449:ILE:HB	2.01	0.42
1:I:85:HIS:ND1	1:I:242:VAL:O	2.37	0.42
1:I:359:ILE:HD13	1:I:466:GLU:HB2	2.02	0.42
1:I:292:VAL:HB	1:I:449:ILE:HB	2.01	0.42
1:I:63:THR:O	1:I:208:VAL:HA	2.18	0.42
1:A:335:LYS:O	1:A:339:ASN:N	2.48	0.42
1:A:223:PHE:CE2	1:A:490:LYS:HB3	2.54	0.42
3:C:18:LEU:HD11	3:C:20:LEU:HD21	2.01	0.42
1:I:231:LYS:HD3	1:I:231:LYS:H	1.85	0.42
1:A:198:THR:O	1:I:312:PRO:HA	2.19	0.42
1:A:292:VAL:HB	1:A:449:ILE:HB	2.01	0.42
2:B:47:ILE:HD12	2:B:47:ILE:HG23	1.81	0.42
1:I:223:PHE:CE2	1:I:490:LYS:HB3	2.54	0.42
1:A:330:HIS:CE1	1:A:415:THR:HG21	2.54	0.42
1:E:231:LYS:HD3	1:E:231:LYS:H	1.85	0.42
1:E:453:ILE:O	1:E:454:LEU:HD23	2.19	0.42
1:E:223:PHE:CE2	1:E:490:LYS:HB3	2.54	0.42
1:E:44:VAL:HB	1:E:492:GLU:HB2	2.01	0.42
1:I:93:PHE:HD2	1:I:239:CYS:HB3	1.84	0.42
1:A:298:ARG:HG2	1:A:383:PHE:HZ	1.82	0.42
1:A:44:VAL:HB	1:A:492:GLU:HB2	2.01	0.42
1:A:93:PHE:HD2	1:A:239:CYS:HB3	1.84	0.42
1:E:54:CYS:HA	1:E:216:HIS:O	2.20	0.42
1:I:330:HIS:CE1	1:I:415:THR:HG21	2.54	0.42
4:D:11:THR:HG22	4:D:72:LYS:HA	2.02	0.41
4:D:157:TRP:CD1	4:D:174:ILE:HD12	2.55	0.41
4:D:93:VAL:HG13	4:D:93:VAL:O	2.20	0.41
1:E:330:HIS:CE1	1:E:415:THR:CG2	3.03	0.41
1:I:330:HIS:CE1	1:I:415:THR:CG2	3.03	0.41
1:A:231:LYS:HD3	1:A:231:LYS:H	1.85	0.41
1:I:129:LEU:HG	1:I:159:PHE:HZ	1.84	0.41
1:I:335:LYS:O	1:I:339:ASN:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:385:CYS:O	1:I:387:THR:HG23	2.21	0.41
1:A:370:GLU:HB2	4:D:43:PHE:CE1	2.55	0.41
1:E:104:MET:HG3	1:E:217:TYR:OH	2.19	0.41
1:E:129:LEU:HG	1:E:159:PHE:HZ	1.84	0.41
1:E:161:MET:SD	1:E:172:VAL:HG21	2.61	0.41
1:E:301:ASN:O	1:E:302:ASN:ND2	2.54	0.41
1:E:385:CYS:O	1:E:387:THR:HG23	2.20	0.41
3:C:43:LYS:HB3	3:C:43:LYS:HE3	1.65	0.41
4:D:120:SER:HA	4:D:121:PRO:HD3	1.86	0.41
1:E:359:ILE:HD13	1:E:466:GLU:HB2	2.02	0.41
1:A:301:ASN:O	1:A:302:ASN:ND2	2.54	0.41
1:A:330:HIS:CE1	1:A:415:THR:CG2	3.03	0.41
1:A:359:ILE:HD13	1:A:466:GLU:HB2	2.02	0.41
1:A:61:TYR:HB3	1:A:62:GLU:H	1.53	0.41
4:D:12:VAL:HG22	4:D:13:GLU:N	2.35	0.41
1:I:54:CYS:HA	1:I:216:HIS:O	2.20	0.41
1:I:104:MET:HG3	1:I:217:TYR:OH	2.19	0.41
1:I:44:VAL:HB	1:I:492:GLU:HB2	2.01	0.41
3:C:1:GLN:CD	3:C:1:GLN:H3	2.24	0.41
4:D:121:PRO:HA	4:D:122:PRO:HD3	1.97	0.41
1:I:62:GLU:HB3	1:I:63:THR:H	1.67	0.41
1:A:54:CYS:HA	1:A:216:HIS:O	2.20	0.41
1:A:359:ILE:HD12	1:A:468:PHE:CE1	2.51	0.41
1:I:161:MET:SD	1:I:172:VAL:HG21	2.61	0.41
1:I:56:SER:O	1:I:57:ASP:HB2	2.21	0.41
4:D:13:GLU:HG3	4:D:70:ILE:HG22	2.03	0.41
1:E:83:GLU:HA	1:E:244:THR:O	2.21	0.41
1:E:335:LYS:HE2	1:E:339:ASN:ND2	2.36	0.41
1:A:325:ASP:C	3:C:100(E):VAL:HG21	2.39	0.40
1:A:385:CYS:O	1:A:387:THR:HG23	2.21	0.40
3:C:197:ASN:OD1	3:C:199:LYS:HG3	2.21	0.40
1:I:301:ASN:O	1:I:302:ASN:ND2	2.54	0.40
1:A:161:MET:SD	1:A:172:VAL:HG21	2.61	0.40
1:A:344:LYS:HA	1:A:347:LYS:HB2	2.03	0.40
1:E:53:PHE:CB	1:E:218:CYS:HB2	2.51	0.40
1:I:335:LYS:HA	1:I:338:TRP:HB3	2.03	0.40
1:A:231:LYS:HB2	1:A:231:LYS:NZ	2.36	0.40
2:B:47:ILE:HD13	2:B:47:ILE:HA	1.87	0.40
3:C:117:PRO:HB3	3:C:143:TYR:HB3	2.03	0.40
3:C:36:TRP:O	3:C:48:ILE:HB	2.21	0.40
1:E:342:LEU:HB3	1:E:395:TRP:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:335:LYS:HE2	1:I:339:ASN:ND2	2.36	0.40
1:I:342:LEU:HB3	1:I:395:TRP:HE1	1.87	0.40
1:I:440:GLN:HB3	1:I:441:GLY:H	1.53	0.40
1:I:62:GLU:O	1:I:63:THR:OG1	2.35	0.40
1:A:83:GLU:HA	1:A:244:THR:O	2.21	0.40
1:E:298:ARG:H	1:E:298:ARG:HG3	1.58	0.40
1:I:104:MET:HG3	1:I:217:TYR:CZ	2.57	0.40
1:I:292:VAL:HG11	1:I:338:TRP:HE3	1.87	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	414/448 (92%)	349 (84%)	51 (12%)	14 (3%)	4	4
1	E	414/448 (92%)	348 (84%)	52 (13%)	14 (3%)	4	4
1	I	414/448 (92%)	349 (84%)	51 (12%)	14 (3%)	4	4
2	B	198/207 (96%)	191 (96%)	7 (4%)	0	100	100
3	C	220/232 (95%)	213 (97%)	6 (3%)	1 (0%)	32	32
4	D	173/175 (99%)	158 (91%)	15 (9%)	0	100	100
All	All	1833/1958 (94%)	1608 (88%)	182 (10%)	43 (2%)	11	7

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	83	GLU
1	A	323	ILE
1	A	429	ARG

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Mol	Chain	Res	Type
1	E	57	ASP
1	E	83	GLU
1	E	323	ILE
1	E	429	ARG
1	I	57	ASP
1	I	83	GLU
1	I	323	ILE
1	I	429	ARG
1	A	195	ASN
1	A	322	ILE
3	C	189	THR
1	E	195	ASN
1	E	322	ILE
1	I	195	ASN
1	I	322	ILE
1	A	56	SER
1	E	56	SER
1	I	56	SER
1	A	63	THR
1	A	220	PRO
1	E	63	THR
1	E	220	PRO
1	I	63	THR
1	I	220	PRO
1	A	84	ILE
1	A	118	PRO
1	E	84	ILE
1	E	118	PRO
1	I	84	ILE
1	I	118	PRO
1	A	89	VAL
1	A	437	PRO
1	E	89	VAL
1	E	437	PRO
1	I	89	VAL
1	I	437	PRO
1	A	442	VAL
1	E	442	VAL
1	I	442	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	317/400 (79%)	293 (92%)	24 (8%)	15	15
1	E	317/400 (79%)	293 (92%)	24 (8%)	15	15
1	I	317/400 (79%)	293 (92%)	24 (8%)	15	15
2	B	171/176 (97%)	164 (96%)	7 (4%)	35	35
3	C	196/202 (97%)	189 (96%)	7 (4%)	40	40
4	D	159/159 (100%)	154 (97%)	5 (3%)	45	45
All	All	1477/1737 (85%)	1386 (94%)	91 (6%)	26	21

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	53	PHE
1	A	61	TYR
1	A	75	VAL
1	A	90	THR
1	A	100	MET
1	A	107	ASP
1	A	125	LEU
1	A	156	ASN
1	A	197	ASN
1	A	226	LEU
1	A	231	LYS
1	A	277	ILE
1	A	298	ARG
1	A	330	HIS
1	A	357	THR
1	A	369	LEU
1	A	374	HIS
1	A	382	PHE
1	A	386	ASN
1	A	399	THR
1	A	412	ASP

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Mol	Chain	Res	Type
1	A	414	ILE
1	A	467	THR
2	B	13	VAL
2	B	17	GLN
2	B	31	ARG
2	B	130	LYS
2	B	136	LEU
2	B	161	GLU
2	B	164	THR
3	C	1	GLN
3	C	16	GLU
3	C	69	LEU
3	C	70	SER
3	C	71	LEU
3	C	181	THR
3	C	191	THR
4	D	63	ASP
4	D	119	GLU
4	D	134	ARG
4	D	152	GLN
4	D	162	LEU
1	E	47	ASP
1	E	53	PHE
1	E	61	TYR
1	E	75	VAL
1	E	90	THR
1	E	100	MET
1	E	107	ASP
1	E	125	LEU
1	E	156	ASN
1	E	197	ASN
1	E	226	LEU
1	E	231	LYS
1	E	277	ILE
1	E	298	ARG
1	E	330	HIS
1	E	357	THR
1	E	369	LEU
1	E	374	HIS
1	E	382	PHE
1	E	386	ASN
1	E	399	THR

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Mol	Chain	Res	Type
1	E	412	ASP
1	E	414	ILE
1	E	467	THR
1	I	47	ASP
1	I	53	PHE
1	I	61	TYR
1	I	75	VAL
1	I	90	THR
1	I	100	MET
1	I	107	ASP
1	I	125	LEU
1	I	156	ASN
1	I	197	ASN
1	I	226	LEU
1	I	231	LYS
1	I	277	ILE
1	I	298	ARG
1	I	330	HIS
1	I	357	THR
1	I	369	LEU
1	I	374	HIS
1	I	382	PHE
1	I	386	ASN
1	I	399	THR
1	I	412	ASP
1	I	414	ILE
1	I	467	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	280	ASN
1	A	330	HIS
1	A	374	HIS
1	A	386	ASN
4	D	40	GLN
4	D	103	ASN
4	D	112	GLN
1	E	130	GLN
1	E	330	HIS
1	E	374	HIS

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Mol	Chain	Res	Type
1	E	386	ASN
1	I	130	GLN
1	I	289	ASN
1	I	330	HIS
1	I	374	HIS
1	I	386	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

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.