



Full wwPDB EM Validation Report ⓘ

Feb 11, 2024 – 09:49 AM EST

PDB ID : 3BYH
Title : Model of actin-fimbrin ABD2 complex
Authors : Galkin, V.E.; Orlova, A.; Cherepanova, O.; Lebart, M.C.; Egelman, E.H.
Deposited on : 2008-01-16
Resolution : 12.00 Å(reported)
Based on initial models : 1PXY, 2BTF

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

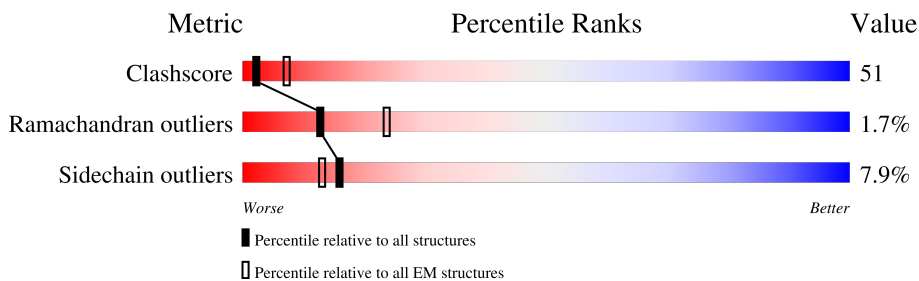
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	374	 47% 40% 10% .
2	B	231	 61% 37% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4795 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 Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	374	2917	1845	490	560	22	0	0

- Molecule 2 is a protein called fimbrin ABD2.

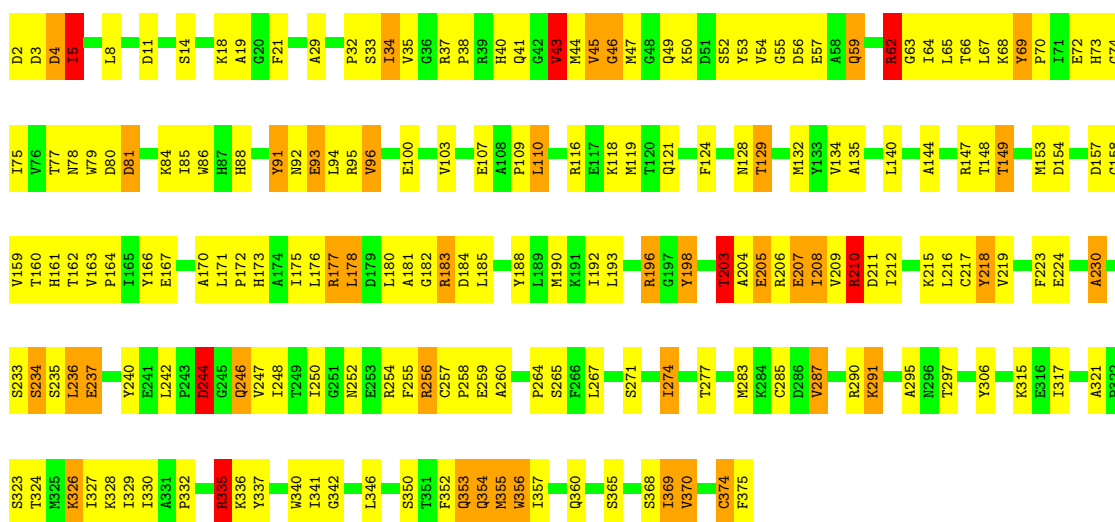
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	231	1878	1207	328	332	11	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

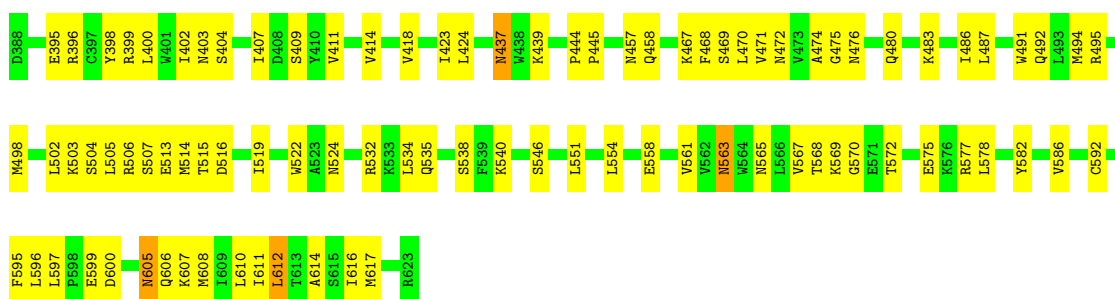
- Molecule 1: Actin

Chain A: 



- Molecule 2: fimbrin ABD2

Chain B: 



4 Data and refinement statistics

Xtrriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 12.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-12.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4795	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.00	0/2976	1.94	86/4022 (2.1%)
2	B	0.29	0/1912	0.50	0/2580
All	All	0.80	0/4888	1.55	86/6602 (1.3%)

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

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	356	TRP	CD1-CG-CD2	13.46	117.06	106.30
1	A	5	ILE	CA-C-N	-11.79	91.26	117.20
1	A	210	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	A	356	TRP	CB-CG-CD1	-9.89	114.15	127.00
1	A	132	MET	CA-CB-CG	9.67	129.74	113.30
1	A	356	TRP	CE2-CD2-CG	-9.50	99.70	107.30
1	A	290	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	A	62	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	79	TRP	CD1-CG-CD2	9.18	113.65	106.30
1	A	62	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	A	116	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	A	356	TRP	CG-CD1-NE1	-8.91	101.19	110.10
1	A	356	TRP	CG-CD2-CE3	8.85	141.87	133.90
1	A	196	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	A	4	ASP	CA-C-N	-8.70	98.06	117.20
1	A	256	ARG	NE-CZ-NH1	8.14	124.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	A	79	TRP	CE2-CD2-CG	-7.87	101.01	107.30
1	A	190	MET	CA-CB-CG	7.84	126.64	113.30
1	A	217	CYS	CA-CB-SG	-7.74	100.07	114.00
1	A	340	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	A	375	PHE	N-CA-C	7.69	131.75	111.00
1	A	69	TYR	CB-CG-CD2	-7.49	116.50	121.00
1	A	86	TRP	CD1-CG-CD2	7.34	112.17	106.30
1	A	183	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	A	188	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	A	37	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	4	ASP	N-CA-C	-7.05	91.98	111.00
1	A	86	TRP	CG-CD2-CE3	7.02	140.22	133.90
1	A	370	VAL	CB-CA-C	-7.01	98.09	111.40
1	A	218	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	A	47	MET	CA-CB-CG	6.81	124.87	113.30
1	A	230	ALA	N-CA-C	-6.69	92.95	111.00
1	A	163	VAL	CG1-CB-CG2	-6.68	100.21	110.90
1	A	132	MET	CG-SD-CE	-6.56	89.70	100.20
1	A	5	ILE	O-C-N	6.51	133.12	122.70
1	A	91	TYR	CB-CG-CD2	-6.34	117.20	121.00
1	A	5	ILE	CA-CB-CG1	-6.21	99.20	111.00
1	A	43	VAL	CA-CB-CG2	-6.21	101.59	110.90
1	A	340	TRP	CE2-CD2-CG	-6.18	102.35	107.30
1	A	62	ARG	CA-CB-CG	6.17	126.98	113.40
1	A	315	LYS	CA-CB-CG	6.13	126.88	113.40
1	A	224	GLU	CA-CB-CG	5.94	126.48	113.40
1	A	86	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	A	235	SER	N-CA-CB	-5.91	101.63	110.50
1	A	129	THR	CA-CB-CG2	-5.91	104.12	112.40
1	A	277	THR	CA-CB-CG2	5.91	120.67	112.40
1	A	147	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	147	ARG	CB-CG-CD	-5.85	96.40	111.60
1	A	81	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	116	ARG	CG-CD-NE	5.82	124.03	111.80
1	A	4	ASP	O-C-N	5.82	132.01	122.70
1	A	356	TRP	CD1-NE1-CE2	5.77	114.19	109.00
1	A	374	CYS	C-N-CA	5.76	136.10	121.70
1	A	218	TYR	CB-CG-CD1	5.65	124.39	121.00
1	A	147	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	256	ARG	CA-CB-CG	5.59	125.70	113.40
1	A	274	ILE	CA-CB-CG1	-5.48	100.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	GLN	N-CA-C	-5.45	96.27	111.00
1	A	323	SER	N-CA-CB	-5.43	102.36	110.50
1	A	353	GLN	CB-CG-CD	5.37	125.55	111.60
1	A	356	TRP	CB-CA-C	-5.34	99.72	110.40
1	A	5	ILE	CA-C-O	5.33	131.30	120.10
1	A	37	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	337	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	A	198	TYR	CB-CG-CD2	-5.29	117.82	121.00
1	A	254	ARG	CB-CG-CD	-5.27	97.91	111.60
1	A	45	VAL	CA-C-N	-5.25	105.70	116.20
1	A	44	MET	CG-SD-CE	-5.24	91.81	100.20
1	A	254	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	237	GLU	CA-CB-CG	5.22	124.89	113.40
1	A	147	ARG	CA-CB-CG	5.22	124.88	113.40
1	A	335	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	205	GLU	CA-CB-CG	5.21	124.86	113.40
1	A	43	VAL	CA-CB-CG1	5.14	118.61	110.90
1	A	329	ILE	CG1-CB-CG2	-5.14	100.09	111.40
1	A	119	MET	CA-CB-CG	5.08	121.94	113.30
1	A	340	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	A	110	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	326	LYS	N-CA-C	-5.05	97.36	111.00
1	A	237	GLU	CB-CG-CD	5.03	127.78	114.20
1	A	79	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	A	11	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	287	VAL	CG1-CB-CG2	-5.02	102.87	110.90
1	A	192	ILE	CA-CB-CG1	5.01	120.53	111.00
1	A	283	MET	CA-CB-CG	-5.01	104.78	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ASP	Mainchain

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	2917	0	2863	321	0
2	B	1878	0	1933	212	0
All	All	4795	0	4796	485	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 51.

All (485) 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:62:ARG:CG	1:A:204:ALA:HA	1.19	1.67
1:A:35:VAL:HB	1:A:70:PRO:CD	1.09	1.54
1:A:35:VAL:CB	1:A:70:PRO:HD3	1.09	1.54
2:B:498:MET:CE	2:B:610:LEU:HD22	1.13	1.54
2:B:498:MET:CG	2:B:610:LEU:HD13	1.31	1.54
2:B:498:MET:CE	2:B:610:LEU:CD2	1.83	1.54
1:A:62:ARG:HG2	1:A:204:ALA:CA	1.06	1.50
2:B:494:MET:CE	2:B:608:MET:HE1	1.45	1.47
1:A:35:VAL:HG21	1:A:70:PRO:CG	1.44	1.47
2:B:498:MET:SD	2:B:610:LEU:HD22	1.54	1.46
1:A:65:LEU:H	1:A:203:THR:CG2	1.29	1.42
1:A:65:LEU:N	1:A:203:THR:HG21	1.15	1.42
1:A:95:ARG:O	2:B:495:ARG:CZ	1.66	1.41
1:A:95:ARG:HH11	2:B:492:GLN:NE2	1.16	1.40
2:B:400:LEU:HD11	2:B:597:LEU:CD2	1.52	1.38
2:B:502:LEU:HB3	2:B:515:THR:C	1.45	1.33
1:A:35:VAL:CG2	1:A:85:ILE:HD11	1.55	1.33
1:A:35:VAL:CG2	1:A:70:PRO:CG	2.08	1.31
2:B:494:MET:HE2	2:B:608:MET:CE	1.61	1.30
1:A:110:LEU:HD11	1:A:176:LEU:O	1.21	1.29
2:B:502:LEU:CD2	2:B:519:ILE:HD12	1.62	1.28
1:A:62:ARG:O	1:A:203:THR:HG22	1.23	1.28
2:B:400:LEU:CD1	2:B:597:LEU:HG	1.63	1.27
2:B:502:LEU:HD23	2:B:519:ILE:CD1	1.64	1.27
1:A:95:ARG:O	2:B:495:ARG:NH1	1.64	1.27
2:B:400:LEU:O	2:B:595:PHE:CB	1.82	1.26
1:A:72:GLU:O	1:A:158:GLY:HA3	1.31	1.26
1:A:63:GLY:CA	1:A:204:ALA:H	1.49	1.25
1:A:65:LEU:N	1:A:203:THR:CG2	1.88	1.25
1:A:68:LYS:HE2	1:A:78:ASN:CB	1.64	1.25
1:A:73:HIS:CE1	1:A:184:ASP:H	1.54	1.24
1:A:73:HIS:CE1	1:A:181:ALA:O	1.89	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:SER:HB3	1:A:81:ASP:OD1	1.34	1.22
2:B:400:LEU:CD1	2:B:597:LEU:CD2	2.19	1.21
1:A:74:GLY:N	1:A:158:GLY:N	1.89	1.20
2:B:498:MET:HE1	2:B:610:LEU:CD2	1.52	1.20
1:A:63:GLY:CA	1:A:204:ALA:N	2.01	1.20
2:B:502:LEU:CD2	2:B:519:ILE:CD1	2.17	1.20
2:B:498:MET:CG	2:B:610:LEU:CD1	2.20	1.19
1:A:73:HIS:O	1:A:158:GLY:N	1.76	1.18
1:A:72:GLU:O	1:A:158:GLY:CA	1.91	1.17
2:B:400:LEU:O	2:B:595:PHE:HB3	1.38	1.17
1:A:63:GLY:N	1:A:204:ALA:N	1.90	1.17
1:A:35:VAL:CB	1:A:70:PRO:CD	1.84	1.16
2:B:400:LEU:CD1	2:B:597:LEU:CG	2.24	1.15
1:A:110:LEU:HD13	1:A:177:ARG:HA	1.18	1.14
2:B:400:LEU:HB3	2:B:595:PHE:O	1.46	1.14
2:B:502:LEU:HD21	2:B:519:ILE:HD12	1.15	1.14
1:A:35:VAL:CB	1:A:70:PRO:CG	2.25	1.13
1:A:35:VAL:CG2	1:A:70:PRO:HG2	1.72	1.13
1:A:109:PRO:O	1:A:161:HIS:ND1	1.82	1.13
2:B:400:LEU:HD12	2:B:597:LEU:HG	1.28	1.13
2:B:502:LEU:HD22	2:B:515:THR:O	1.45	1.12
1:A:95:ARG:NH1	2:B:492:GLN:NE2	1.96	1.12
1:A:95:ARG:NH1	2:B:468:PHE:CG	2.18	1.12
2:B:502:LEU:HB3	2:B:515:THR:CA	1.80	1.11
1:A:69:TYR:O	1:A:72:GLU:HA	1.50	1.11
1:A:53:TYR:CD1	2:B:472:ASN:OD1	2.01	1.11
1:A:62:ARG:O	1:A:203:THR:CG2	1.99	1.10
1:A:35:VAL:HG22	1:A:85:ILE:HD11	1.17	1.09
1:A:64:ILE:C	1:A:203:THR:HG21	1.71	1.09
1:A:54:VAL:HG21	1:A:85:ILE:HG12	1.33	1.09
1:A:35:VAL:CG2	1:A:85:ILE:CD1	2.30	1.09
1:A:73:HIS:NE2	1:A:184:ASP:N	2.00	1.08
1:A:35:VAL:HG11	1:A:70:PRO:HG3	1.19	1.08
1:A:110:LEU:CD1	1:A:176:LEU:O	2.01	1.07
2:B:498:MET:HG2	2:B:610:LEU:HD13	1.10	1.06
2:B:504:SER:N	2:B:514:MET:HB2	1.71	1.06
1:A:68:LYS:HE2	1:A:78:ASN:HB3	1.38	1.05
1:A:35:VAL:CG2	1:A:70:PRO:CD	2.30	1.04
2:B:498:MET:HE2	2:B:610:LEU:CD2	1.82	1.04
1:A:35:VAL:CG1	1:A:70:PRO:HG3	1.87	1.04
1:A:53:TYR:HD1	2:B:472:ASN:OD1	1.33	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:NH1	2:B:468:PHE:CD2	2.26	1.03
1:A:88:HIS:CE1	2:B:471:VAL:HG22	1.93	1.03
2:B:494:MET:CE	2:B:608:MET:CE	2.25	1.03
2:B:400:LEU:HD11	2:B:597:LEU:HD21	1.03	1.02
1:A:68:LYS:HE2	1:A:78:ASN:HB2	1.33	1.02
2:B:498:MET:SD	2:B:610:LEU:CD2	2.38	1.02
2:B:506:ARG:H	2:B:514:MET:N	1.32	1.02
1:A:95:ARG:HH11	2:B:492:GLN:CD	1.60	1.01
1:A:69:TYR:O	1:A:157:ASP:OD2	1.79	0.99
1:A:73:HIS:CD2	1:A:184:ASP:OD1	2.14	0.99
2:B:498:MET:HG3	2:B:610:LEU:HD13	1.41	0.98
2:B:498:MET:CE	2:B:610:LEU:HD21	1.89	0.98
2:B:498:MET:SD	2:B:610:LEU:HD13	2.02	0.98
2:B:502:LEU:CB	2:B:515:THR:C	2.32	0.97
1:A:73:HIS:ND1	1:A:181:ALA:C	2.17	0.97
2:B:498:MET:HG3	2:B:610:LEU:CD1	1.93	0.96
2:B:506:ARG:N	2:B:514:MET:N	2.11	0.96
1:A:73:HIS:CE1	1:A:184:ASP:N	2.27	0.95
1:A:73:HIS:CE1	1:A:181:ALA:C	2.40	0.95
1:A:62:ARG:CB	1:A:204:ALA:HA	1.97	0.94
1:A:62:ARG:CG	1:A:204:ALA:CA	2.02	0.94
1:A:43:VAL:HG21	1:A:49:GLN:HA	1.47	0.94
2:B:498:MET:HE2	2:B:610:LEU:HD21	1.43	0.93
1:A:68:LYS:CE	1:A:78:ASN:HB2	1.99	0.93
1:A:95:ARG:NH2	2:B:468:PHE:CE2	2.36	0.93
2:B:498:MET:HE1	2:B:610:LEU:HD22	1.08	0.92
2:B:507:SER:N	2:B:513:GLU:CG	2.32	0.92
2:B:502:LEU:HD23	2:B:519:ILE:CG1	2.01	0.91
2:B:519:ILE:HG23	2:B:617:MET:HE3	1.52	0.91
2:B:502:LEU:HD23	2:B:519:ILE:HD11	1.52	0.90
1:A:96:VAL:HA	2:B:495:ARG:NH2	1.86	0.90
1:A:95:ARG:HH21	2:B:492:GLN:C	1.65	0.90
1:A:62:ARG:HG2	1:A:204:ALA:C	1.91	0.90
1:A:73:HIS:NE2	1:A:184:ASP:OD1	2.04	0.90
1:A:69:TYR:O	1:A:72:GLU:CA	2.20	0.90
2:B:400:LEU:O	2:B:595:PHE:HB2	1.71	0.90
2:B:502:LEU:CD2	2:B:519:ILE:CG1	2.51	0.88
2:B:469:SER:H	2:B:492:GLN:HE22	1.20	0.88
1:A:73:HIS:C	1:A:158:GLY:N	0.83	0.88
1:A:91:TYR:O	2:B:469:SER:N	2.07	0.88
1:A:110:LEU:HD21	1:A:176:LEU:C	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD22	1:A:177:ARG:CB	2.05	0.87
2:B:502:LEU:HD21	2:B:519:ILE:CD1	1.96	0.86
1:A:73:HIS:CG	1:A:181:ALA:HB3	2.10	0.86
1:A:109:PRO:O	1:A:161:HIS:CE1	2.27	0.86
2:B:400:LEU:HD11	2:B:597:LEU:CG	1.93	0.86
2:B:403:ASN:HD21	2:B:411:VAL:H	1.22	0.86
1:A:110:LEU:CD2	1:A:175:ILE:HG22	2.06	0.85
1:A:68:LYS:HB2	1:A:70:PRO:N	1.90	0.85
1:A:35:VAL:HG23	1:A:85:ILE:HD11	1.58	0.85
1:A:95:ARG:NH2	2:B:468:PHE:CZ	2.45	0.85
1:A:35:VAL:HG21	1:A:70:PRO:HG2	0.86	0.85
1:A:91:TYR:HB3	2:B:467:LYS:O	1.75	0.84
1:A:72:GLU:HA	1:A:157:ASP:OD2	1.75	0.84
1:A:14:SER:CB	1:A:157:ASP:HB2	2.08	0.84
2:B:400:LEU:CD1	2:B:597:LEU:HD21	1.95	0.84
1:A:14:SER:OG	1:A:157:ASP:CB	2.26	0.84
1:A:54:VAL:CG2	1:A:85:ILE:HG12	2.08	0.84
1:A:64:ILE:CA	1:A:203:THR:HG21	2.07	0.84
2:B:502:LEU:CD2	2:B:515:THR:O	2.26	0.84
2:B:502:LEU:HB3	2:B:516:ASP:N	1.91	0.83
1:A:95:ARG:NH1	2:B:492:GLN:CD	2.17	0.83
1:A:35:VAL:CA	1:A:70:PRO:HD3	2.08	0.83
1:A:68:LYS:HZ3	1:A:70:PRO:N	1.77	0.83
1:A:35:VAL:HG22	1:A:85:ILE:CD1	2.04	0.82
2:B:437:ASN:H	2:B:458:GLN:HE22	1.23	0.82
1:A:95:ARG:NH2	2:B:492:GLN:C	2.32	0.81
2:B:498:MET:HG2	2:B:610:LEU:CD1	1.96	0.81
1:A:110:LEU:CD1	1:A:177:ARG:HA	2.08	0.81
1:A:73:HIS:HD1	1:A:182:GLY:N	1.80	0.80
1:A:35:VAL:HG21	1:A:70:PRO:HG3	1.62	0.80
1:A:88:HIS:CE1	2:B:471:VAL:CG2	2.65	0.80
2:B:400:LEU:CB	2:B:595:PHE:O	2.29	0.80
1:A:14:SER:OG	1:A:157:ASP:HB3	1.81	0.79
1:A:75:ILE:HD11	1:A:159:VAL:CG1	2.12	0.79
2:B:502:LEU:HD22	2:B:515:THR:C	2.01	0.79
2:B:502:LEU:CD2	2:B:519:ILE:HG13	2.12	0.79
2:B:507:SER:N	2:B:513:GLU:HG3	1.81	0.79
1:A:62:ARG:O	1:A:203:THR:C	2.21	0.79
1:A:64:ILE:N	1:A:203:THR:HG21	1.90	0.79
1:A:73:HIS:CB	1:A:181:ALA:HB3	2.12	0.79
1:A:33:SER:N	1:A:34:ILE:N	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:C	1:A:203:THR:C	2.41	0.78
1:A:73:HIS:HB3	1:A:181:ALA:HB3	1.65	0.78
1:A:110:LEU:HD22	1:A:177:ARG:CA	2.14	0.78
1:A:62:ARG:O	1:A:203:THR:CB	2.31	0.78
1:A:109:PRO:HG2	1:A:154:ASP:CG	2.03	0.78
1:A:65:LEU:H	1:A:203:THR:HG22	1.43	0.78
2:B:403:ASN:O	2:B:595:PHE:CE2	2.37	0.78
1:A:110:LEU:CD2	1:A:176:LEU:C	2.52	0.77
1:A:14:SER:CB	1:A:157:ASP:CB	2.63	0.77
2:B:519:ILE:HA	2:B:617:MET:HE1	1.66	0.77
1:A:75:ILE:HD11	1:A:159:VAL:HG11	1.66	0.77
2:B:502:LEU:HD23	2:B:519:ILE:HG13	1.66	0.77
1:A:72:GLU:C	1:A:158:GLY:CA	2.47	0.77
1:A:35:VAL:CB	1:A:70:PRO:HG3	2.10	0.76
2:B:498:MET:SD	2:B:611:ILE:HD13	2.26	0.76
1:A:32:PRO:O	1:A:55:GLY:N	2.18	0.76
2:B:498:MET:SD	2:B:610:LEU:CG	2.75	0.75
2:B:498:MET:SD	2:B:611:ILE:CD1	2.74	0.75
2:B:546:SER:HB2	2:B:570:GLY:HA3	1.69	0.75
1:A:95:ARG:HH12	2:B:468:PHE:CB	2.00	0.74
1:A:95:ARG:NH2	2:B:492:GLN:O	2.19	0.74
1:A:110:LEU:HD22	1:A:177:ARG:N	2.02	0.74
1:A:212:ILE:HG23	1:A:216:LEU:HD12	1.68	0.74
2:B:502:LEU:CB	2:B:516:ASP:N	2.50	0.73
2:B:502:LEU:HB3	2:B:515:THR:HA	1.70	0.73
1:A:3:ASP:OD2	2:B:606:GLN:CD	2.27	0.73
2:B:498:MET:SD	2:B:610:LEU:CD1	2.71	0.73
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.72	0.72
1:A:317:ILE:HG22	1:A:327:ILE:HD13	1.69	0.72
2:B:400:LEU:HD13	2:B:597:LEU:CD2	2.16	0.72
1:A:14:SER:OG	1:A:157:ASP:HB2	1.90	0.72
2:B:503:LYS:C	2:B:514:MET:HB2	2.09	0.72
1:A:109:PRO:C	1:A:161:HIS:ND1	2.35	0.72
1:A:73:HIS:HD1	1:A:181:ALA:C	1.93	0.72
1:A:95:ARG:O	2:B:495:ARG:NE	2.21	0.72
2:B:507:SER:H	2:B:513:GLU:HG3	1.55	0.71
1:A:72:GLU:O	1:A:158:GLY:HA2	1.90	0.71
1:A:3:ASP:OD2	2:B:606:GLN:OE1	2.08	0.71
1:A:205:GLU:HA	1:A:208:ILE:HB	1.72	0.71
2:B:400:LEU:CD1	2:B:597:LEU:HD23	2.21	0.71
1:A:52:SER:CB	1:A:81:ASP:OD1	2.27	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:MET:SD	2:B:610:LEU:HB3	2.30	0.71
1:A:160:THR:HG21	1:A:274:ILE:HD11	1.70	0.71
1:A:63:GLY:N	1:A:203:THR:C	2.42	0.70
1:A:110:LEU:HD13	1:A:177:ARG:CA	2.10	0.70
1:A:62:ARG:C	1:A:204:ALA:N	2.45	0.69
1:A:73:HIS:NE2	1:A:183:ARG:HB3	2.07	0.69
1:A:35:VAL:HB	1:A:70:PRO:N	2.04	0.69
1:A:110:LEU:HB3	1:A:177:ARG:HB2	1.73	0.69
2:B:506:ARG:N	2:B:514:MET:CA	2.56	0.69
1:A:68:LYS:CB	1:A:70:PRO:N	2.55	0.69
2:B:476:ASN:O	2:B:480:GLN:HG3	1.93	0.68
1:A:110:LEU:HD22	1:A:177:ARG:HB2	1.75	0.68
1:A:110:LEU:HD21	1:A:175:ILE:HG22	1.76	0.68
1:A:240:TYR:HB3	1:A:248:ILE:HD12	1.74	0.68
1:A:14:SER:HB3	1:A:157:ASP:CB	2.24	0.67
2:B:457:ASN:ND2	2:B:475:GLY:H	1.92	0.67
2:B:495:ARG:HB2	2:B:607:LYS:HE3	1.76	0.67
1:A:33:SER:H	1:A:34:ILE:N	1.92	0.67
1:A:110:LEU:HD23	1:A:175:ILE:HG22	1.76	0.66
2:B:498:MET:HG3	2:B:610:LEU:HD11	1.77	0.66
1:A:73:HIS:HE1	1:A:181:ALA:O	1.72	0.66
2:B:400:LEU:O	2:B:595:PHE:CG	2.49	0.66
1:A:63:GLY:N	1:A:204:ALA:H	1.73	0.66
2:B:400:LEU:HD13	2:B:597:LEU:HD23	1.78	0.65
2:B:418:VAL:CG2	2:B:424:LEU:HG	2.26	0.65
1:A:74:GLY:H	1:A:157:ASP:HB3	1.62	0.65
1:A:62:ARG:C	1:A:203:THR:CG2	2.65	0.65
2:B:558:GLU:O	2:B:561:VAL:HG22	1.97	0.65
2:B:506:ARG:H	2:B:514:MET:CA	2.09	0.65
1:A:68:LYS:HD3	1:A:77:THR:OG1	1.97	0.65
1:A:14:SER:HB3	1:A:157:ASP:CG	2.18	0.64
1:A:63:GLY:HA3	1:A:204:ALA:H	1.58	0.64
1:A:95:ARG:HG3	2:B:491:TRP:CD1	2.32	0.64
1:A:35:VAL:HG21	1:A:85:ILE:CD1	2.24	0.64
1:A:63:GLY:HA2	1:A:204:ALA:N	1.61	0.64
1:A:68:LYS:HD2	1:A:70:PRO:HA	1.78	0.64
1:A:64:ILE:N	1:A:203:THR:CG2	2.34	0.64
2:B:437:ASN:C	2:B:437:ASN:HD22	2.01	0.64
1:A:62:ARG:C	1:A:203:THR:HG22	2.14	0.63
1:A:95:ARG:NH1	2:B:468:PHE:CB	2.58	0.63
1:A:73:HIS:NE2	1:A:183:ARG:CB	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:504:SER:N	2:B:514:MET:CB	2.55	0.62
2:B:407:ILE:HG12	2:B:409:SER:H	1.65	0.62
2:B:503:LYS:C	2:B:514:MET:CB	2.67	0.62
1:A:68:LYS:CE	1:A:78:ASN:CB	2.55	0.62
1:A:73:HIS:ND1	1:A:182:GLY:N	2.43	0.62
1:A:92:ASN:HA	2:B:492:GLN:HE22	1.63	0.62
1:A:242:LEU:HD23	1:A:246:GLN:HB3	1.79	0.62
1:A:107:GLU:HG2	1:A:134:VAL:HG12	1.82	0.61
1:A:5:ILE:HD11	1:A:100:GLU:O	2.00	0.61
2:B:400:LEU:C	2:B:595:PHE:HB3	2.19	0.61
1:A:62:ARG:CG	1:A:204:ALA:O	2.48	0.61
1:A:64:ILE:C	1:A:203:THR:CG2	2.53	0.61
1:A:357:ILE:HG23	1:A:369:ILE:HD13	1.83	0.61
1:A:110:LEU:HD21	1:A:176:LEU:O	2.00	0.60
1:A:68:LYS:CD	1:A:77:THR:OG1	2.49	0.60
1:A:59:GLN:O	1:A:62:ARG:HB3	2.02	0.60
2:B:498:MET:HE1	2:B:610:LEU:HD23	1.71	0.60
1:A:3:ASP:OD2	2:B:606:GLN:NE2	2.35	0.60
1:A:330:ILE:HG22	1:A:332:PRO:HD3	1.83	0.60
1:A:67:LEU:HD13	1:A:207:GLU:HG2	1.84	0.60
1:A:64:ILE:CA	1:A:203:THR:CG2	2.76	0.60
1:A:69:TYR:HB2	1:A:157:ASP:OD2	2.01	0.60
1:A:69:TYR:HB3	1:A:157:ASP:OD1	2.01	0.60
2:B:506:ARG:N	2:B:514:MET:HA	2.17	0.60
2:B:507:SER:H	2:B:513:GLU:CG	2.12	0.60
2:B:403:ASN:C	2:B:595:PHE:CE2	2.71	0.59
1:A:73:HIS:ND1	1:A:181:ALA:HB3	2.16	0.59
1:A:67:LEU:CD1	1:A:207:GLU:HG2	2.31	0.59
1:A:81:ASP:HA	1:A:84:LYS:HG2	1.83	0.59
1:A:46:GLY:O	2:B:474:ALA:HB2	2.02	0.59
1:A:62:ARG:HG3	1:A:207:GLU:HB2	1.85	0.59
2:B:395:GLU:HG2	2:B:414:VAL:HG22	1.83	0.59
2:B:522:TRP:CE3	2:B:617:MET:HE2	2.38	0.59
1:A:75:ILE:CG1	1:A:159:VAL:HB	2.32	0.59
1:A:110:LEU:CD2	1:A:177:ARG:N	2.66	0.59
2:B:572:THR:OG1	2:B:575:GLU:HG3	2.03	0.59
1:A:57:GLU:OE2	2:B:471:VAL:HB	2.03	0.58
1:A:237:GLU:HA	1:A:250:ILE:O	2.02	0.58
1:A:75:ILE:HD11	1:A:159:VAL:CB	2.32	0.58
2:B:519:ILE:HA	2:B:617:MET:CE	2.34	0.58
1:A:88:HIS:ND1	2:B:471:VAL:HG13	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:LEU:CD2	2:B:515:THR:C	2.69	0.58
1:A:91:TYR:O	2:B:468:PHE:C	2.42	0.58
2:B:522:TRP:HB3	2:B:617:MET:HE1	1.85	0.58
1:A:218:TYR:O	1:A:255:PHE:HA	2.04	0.57
2:B:437:ASN:ND2	2:B:439:LYS:H	2.02	0.57
2:B:494:MET:SD	2:B:608:MET:CE	2.91	0.57
2:B:534:LEU:HD23	2:B:534:LEU:H	1.69	0.57
1:A:62:ARG:CD	1:A:204:ALA:HA	2.25	0.57
2:B:437:ASN:H	2:B:458:GLN:NE2	1.98	0.57
2:B:494:MET:HE2	2:B:608:MET:HE1	0.65	0.57
1:A:78:ASN:OD1	1:A:81:ASP:HB2	2.05	0.57
1:A:3:ASP:HB2	2:B:606:GLN:HE22	1.70	0.56
1:A:62:ARG:O	1:A:203:THR:CA	2.54	0.56
2:B:399:ARG:HG3	2:B:411:VAL:HG12	1.87	0.56
1:A:260:ALA:HB1	1:A:267:LEU:HG	1.88	0.56
1:A:75:ILE:HD11	1:A:159:VAL:HB	1.87	0.56
2:B:498:MET:SD	2:B:610:LEU:CB	2.93	0.56
1:A:62:ARG:NE	1:A:204:ALA:O	2.40	0.55
1:A:110:LEU:CD2	1:A:176:LEU:O	2.53	0.55
1:A:35:VAL:CG2	1:A:85:ILE:HD12	2.34	0.55
1:A:69:TYR:OH	1:A:210:ARG:HD3	2.06	0.55
2:B:524:ASN:HB3	2:B:535:GLN:OE1	2.06	0.55
2:B:400:LEU:C	2:B:595:PHE:CB	2.72	0.55
1:A:95:ARG:CZ	2:B:468:PHE:CD2	2.89	0.55
2:B:563:ASN:C	2:B:563:ASN:HD22	2.10	0.55
2:B:437:ASN:HD21	2:B:439:LYS:HB3	1.71	0.54
2:B:554:LEU:HD21	2:B:616:ILE:HD12	1.90	0.54
2:B:494:MET:SD	2:B:608:MET:HE3	2.48	0.53
2:B:502:LEU:CG	2:B:515:THR:C	2.76	0.53
2:B:592:CYS:SG	2:B:616:ILE:HD13	2.49	0.53
1:A:95:ARG:NH1	2:B:492:GLN:HE21	1.97	0.52
1:A:35:VAL:HG22	1:A:54:VAL:HG22	1.92	0.52
1:A:135:ALA:HB1	1:A:140:LEU:HD11	1.92	0.52
1:A:62:ARG:CG	1:A:204:ALA:C	2.66	0.52
2:B:398:TYR:O	2:B:402:ILE:HG13	2.10	0.52
1:A:178:LEU:HD13	1:A:274:ILE:HD12	1.91	0.52
1:A:2:ASP:CB	2:B:538:SER:OG	2.58	0.52
1:A:68:LYS:CE	1:A:70:PRO:HA	2.40	0.52
2:B:437:ASN:HD22	2:B:439:LYS:H	1.57	0.52
2:B:519:ILE:HD13	2:B:614:ALA:HB2	1.92	0.52
1:A:8:LEU:HD22	1:A:21:PHE:HE1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:HG2	1:A:204:ALA:N	2.07	0.51
1:A:62:ARG:NH1	1:A:207:GLU:OE1	2.25	0.51
2:B:582:TYR:O	2:B:586:VAL:HG23	2.10	0.51
1:A:35:VAL:HG23	1:A:85:ILE:CD1	2.27	0.51
1:A:352:PHE:HE2	1:A:356:TRP:CZ3	2.29	0.51
2:B:400:LEU:HD13	2:B:597:LEU:CG	2.31	0.51
2:B:400:LEU:HD13	2:B:597:LEU:HG	1.78	0.51
1:A:153:MET:HG2	1:A:162:THR:HG22	1.91	0.51
1:A:14:SER:O	1:A:69:TYR:HA	2.11	0.51
1:A:110:LEU:CD2	1:A:175:ILE:CG2	2.85	0.51
1:A:178:LEU:HD13	1:A:274:ILE:CD1	2.41	0.51
1:A:185:LEU:HD23	1:A:306:TYR:OH	2.11	0.51
2:B:612:LEU:O	2:B:616:ILE:HG12	2.11	0.51
1:A:43:VAL:HG21	1:A:49:GLN:CA	2.32	0.50
2:B:469:SER:C	2:B:470:LEU:HD22	2.31	0.50
1:A:63:GLY:N	1:A:204:ALA:CA	2.73	0.50
1:A:52:SER:OG	1:A:84:LYS:HG3	2.11	0.50
1:A:65:LEU:H	1:A:203:THR:HG21	0.74	0.50
1:A:77:THR:HG21	1:A:183:ARG:NH2	2.27	0.50
1:A:252:ASN:O	1:A:256:ARG:HG3	2.11	0.50
1:A:52:SER:OG	1:A:84:LYS:CB	2.60	0.50
2:B:469:SER:N	2:B:492:GLN:HE22	2.00	0.50
2:B:522:TRP:HB3	2:B:617:MET:CE	2.42	0.50
2:B:546:SER:CB	2:B:570:GLY:HA3	2.40	0.50
1:A:2:ASP:HB2	2:B:538:SER:CB	2.42	0.49
1:A:8:LEU:HD11	1:A:96:VAL:HG11	1.93	0.49
1:A:209:VAL:HA	1:A:212:ILE:HD12	1.95	0.49
1:A:92:ASN:HA	2:B:492:GLN:NE2	2.26	0.49
1:A:35:VAL:CG1	1:A:70:PRO:CG	2.60	0.49
2:B:597:LEU:O	2:B:600:ASP:HB2	2.12	0.49
1:A:95:ARG:CB	2:B:492:GLN:HG2	2.14	0.49
1:A:352:PHE:CD1	1:A:355:MET:SD	3.06	0.49
2:B:563:ASN:HD22	2:B:565:ASN:H	1.60	0.49
1:A:62:ARG:CD	1:A:204:ALA:CA	2.88	0.49
1:A:68:LYS:CD	1:A:70:PRO:HA	2.42	0.49
2:B:418:VAL:HG22	2:B:424:LEU:HG	1.93	0.49
1:A:35:VAL:HG21	1:A:85:ILE:HD12	1.93	0.48
1:A:95:ARG:NH2	2:B:468:PHE:CD2	2.80	0.48
2:B:437:ASN:C	2:B:437:ASN:ND2	2.66	0.48
1:A:32:PRO:O	1:A:54:VAL:CG1	2.61	0.48
1:A:88:HIS:ND1	2:B:471:VAL:CG1	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:TYR:CE2	1:A:210:ARG:HD3	2.48	0.48
1:A:69:TYR:CB	1:A:157:ASP:OD2	2.62	0.48
1:A:144:ALA:HB2	1:A:342:GLY:CA	2.42	0.48
1:A:244:ASP:OD1	1:A:246:GLN:HB2	2.14	0.48
2:B:444:PRO:HA	2:B:445:PRO:C	2.34	0.48
2:B:522:TRP:CD2	2:B:617:MET:HG3	2.49	0.48
1:A:357:ILE:HD11	1:A:374:CYS:SG	2.54	0.48
1:A:68:LYS:HD2	1:A:70:PRO:CA	2.42	0.48
1:A:3:ASP:CG	2:B:606:GLN:HE22	2.17	0.47
1:A:32:PRO:O	1:A:54:VAL:HG13	2.15	0.47
1:A:69:TYR:CB	1:A:157:ASP:OD1	2.61	0.47
2:B:507:SER:N	2:B:513:GLU:HG2	2.24	0.47
1:A:8:LEU:HD22	1:A:21:PHE:CE1	2.50	0.47
1:A:67:LEU:HD13	1:A:207:GLU:CG	2.44	0.47
1:A:73:HIS:CE1	1:A:182:GLY:N	2.83	0.47
1:A:110:LEU:HD21	1:A:176:LEU:N	2.28	0.47
1:A:75:ILE:H	1:A:158:GLY:HA3	1.78	0.47
1:A:211:ASP:O	1:A:215:LYS:HD3	2.14	0.47
1:A:3:ASP:CB	2:B:606:GLN:HE22	2.26	0.47
2:B:605:ASN:C	2:B:605:ASN:HD22	2.18	0.47
1:A:2:ASP:HB3	2:B:538:SER:OG	2.14	0.47
1:A:33:SER:CA	1:A:34:ILE:N	2.76	0.47
1:A:52:SER:OG	1:A:84:LYS:HB2	2.14	0.47
1:A:62:ARG:HH12	1:A:207:GLU:CD	1.79	0.47
2:B:495:ARG:HB2	2:B:607:LYS:CE	2.43	0.47
2:B:457:ASN:HD21	2:B:475:GLY:H	1.61	0.47
2:B:563:ASN:ND2	2:B:565:ASN:H	2.13	0.47
1:A:230:ALA:HA	1:A:236:LEU:HG	1.97	0.47
1:A:69:TYR:CE2	1:A:210:ARG:CD	2.97	0.46
2:B:540:LYS:O	2:B:540:LYS:HG2	2.15	0.46
1:A:68:LYS:HZ3	1:A:70:PRO:CA	2.26	0.46
1:A:73:HIS:C	1:A:157:ASP:N	2.69	0.46
1:A:59:GLN:HE21	1:A:59:GLN:HA	1.81	0.46
1:A:332:PRO:O	1:A:335:ARG:HB3	2.15	0.46
1:A:95:ARG:HB3	2:B:492:GLN:HG2	1.91	0.46
1:A:171:LEU:HB3	1:A:173:HIS:CE1	2.50	0.46
2:B:506:ARG:HD2	2:B:513:GLU:HA	1.33	0.46
1:A:5:ILE:HA	1:A:5:ILE:HD13	1.57	0.46
1:A:65:LEU:N	1:A:203:THR:HG23	2.14	0.46
1:A:72:GLU:HA	1:A:183:ARG:HD3	1.98	0.46
2:B:411:VAL:HG22	2:B:423:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:532:ARG:HB3	2:B:534:LEU:CD2	2.45	0.45
1:A:54:VAL:CG2	1:A:85:ILE:CG1	2.87	0.45
1:A:154:ASP:O	1:A:160:THR:HA	2.16	0.45
2:B:569:LYS:O	2:B:575:GLU:HB3	2.17	0.45
1:A:43:VAL:HG21	1:A:50:LYS:H	1.82	0.45
1:A:295:ALA:O	1:A:328:LYS:HB3	2.16	0.45
1:A:326:LYS:NZ	1:A:328:LYS:HD2	2.31	0.45
1:A:14:SER:HB3	1:A:157:ASP:HB2	1.91	0.45
2:B:596:LEU:HD23	2:B:596:LEU:H	1.81	0.45
1:A:68:LYS:HB2	1:A:68:LYS:HZ3	1.81	0.45
1:A:73:HIS:CD2	1:A:183:ARG:HB3	2.51	0.45
1:A:219:VAL:HG23	1:A:306:TYR:HB3	1.99	0.45
1:A:144:ALA:HB2	1:A:342:GLY:HA2	1.99	0.45
1:A:321:ALA:CB	1:A:327:ILE:HD11	2.46	0.45
2:B:403:ASN:O	2:B:595:PHE:CZ	2.60	0.45
1:A:109:PRO:HG2	1:A:154:ASP:CB	2.46	0.45
2:B:396:ARG:NH2	2:B:599:GLU:HG2	2.32	0.45
1:A:110:LEU:HD13	1:A:160:THR:O	2.17	0.45
1:A:352:PHE:HE2	1:A:356:TRP:CH2	2.34	0.45
1:A:73:HIS:ND1	1:A:181:ALA:CB	2.80	0.44
1:A:75:ILE:CD1	1:A:159:VAL:HB	2.46	0.44
1:A:118:LYS:O	1:A:121:GLN:HB3	2.18	0.44
2:B:404:SER:N	2:B:595:PHE:CD2	2.71	0.44
2:B:494:MET:HE1	2:B:608:MET:CE	2.37	0.44
1:A:59:GLN:HE22	1:A:62:ARG:NH1	2.16	0.44
1:A:354:GLN:O	1:A:355:MET:HB2	2.18	0.44
2:B:505:LEU:HB2	2:B:514:MET:CA	2.33	0.44
1:A:149:THR:HG23	1:A:166:TYR:HA	1.99	0.44
1:A:8:LEU:CD1	1:A:96:VAL:HG11	2.46	0.44
2:B:418:VAL:HG11	2:B:486:ILE:HD13	2.00	0.44
1:A:65:LEU:O	1:A:203:THR:HG22	2.17	0.44
1:A:69:TYR:HB3	1:A:157:ASP:CG	2.39	0.43
1:A:19:ALA:HB1	1:A:94:LEU:HD11	1.99	0.43
2:B:505:LEU:HD12	2:B:514:MET:HG3	1.25	0.43
1:A:29:ALA:HB1	1:A:93:GLU:HG2	2.01	0.43
1:A:45:VAL:HG12	1:A:45:VAL:O	2.19	0.43
1:A:59:GLN:HE22	1:A:62:ARG:HH11	1.67	0.43
2:B:470:LEU:HD22	2:B:470:LEU:N	2.33	0.43
1:A:67:LEU:CD1	1:A:207:GLU:CG	2.97	0.43
1:A:297:THR:O	1:A:330:ILE:N	2.52	0.43
1:A:32:PRO:HG2	1:A:56:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:LEU:O	2:B:514:MET:SD	2.55	0.42
1:A:69:TYR:CB	1:A:157:ASP:CG	2.87	0.42
1:A:124:PHE:O	1:A:128:ASN:HA	2.18	0.42
2:B:498:MET:CE	2:B:611:ILE:HD13	2.49	0.42
1:A:32:PRO:O	1:A:55:GLY:CA	2.67	0.42
2:B:551:LEU:HD13	2:B:567:VAL:CG1	2.49	0.42
2:B:568:THR:HG21	2:B:578:LEU:HD23	2.01	0.42
1:A:166:TYR:CE1	1:A:167:GLU:HG2	2.55	0.42
2:B:483:LYS:O	2:B:487:LEU:HG	2.20	0.42
2:B:403:ASN:ND2	2:B:411:VAL:H	2.03	0.42
2:B:418:VAL:CG1	2:B:486:ILE:HD13	2.50	0.42
2:B:437:ASN:HD21	2:B:439:LYS:CB	2.32	0.42
1:A:95:ARG:CZ	2:B:492:GLN:NE2	2.71	0.42
1:A:170:ALA:O	1:A:172:PRO:HD3	2.19	0.42
1:A:159:VAL:HG21	1:A:177:ARG:HD2	2.01	0.42
1:A:110:LEU:CD2	1:A:161:HIS:NE2	2.38	0.41
1:A:287:VAL:O	1:A:291:LYS:NZ	2.53	0.41
2:B:494:MET:CE	2:B:608:MET:HE3	2.36	0.41
2:B:502:LEU:CB	2:B:515:THR:CA	2.73	0.41
2:B:505:LEU:C	2:B:514:MET:HA	2.38	0.41
1:A:135:ALA:CB	1:A:140:LEU:HD11	2.49	0.41
1:A:264:PRO:HD2	1:A:271:SER:O	2.20	0.41
1:A:73:HIS:HE1	1:A:184:ASP:N	2.05	0.41
1:A:88:HIS:ND1	2:B:469:SER:OG	2.53	0.41
2:B:505:LEU:HB2	2:B:514:MET:HA	2.02	0.41
2:B:505:LEU:HB2	2:B:514:MET:HB3	1.55	0.41
1:A:69:TYR:HE2	1:A:210:ARG:CD	2.34	0.41
1:A:110:LEU:HD21	1:A:176:LEU:CA	2.49	0.41
1:A:164:PRO:HG2	1:A:285:CYS:SG	2.61	0.41
1:A:91:TYR:O	2:B:492:GLN:NE2	2.54	0.41
1:A:223:PHE:CD1	1:A:259:GLU:HG3	2.56	0.41
1:A:193:LEU:O	1:A:198:TYR:HD2	2.03	0.41
1:A:43:VAL:CG2	1:A:50:LYS:H	2.34	0.41
1:A:103:VAL:HG22	1:A:129:THR:HG21	2.02	0.41
1:A:193:LEU:O	1:A:198:TYR:CD2	2.74	0.41
1:A:274:ILE:HD12	1:A:274:ILE:HA	1.85	0.41
2:B:437:ASN:N	2:B:458:GLN:HE22	2.04	0.41
1:A:353:GLN:NE2	1:A:356:TRP:HE1	2.19	0.40
1:A:65:LEU:O	1:A:203:THR:CG2	2.70	0.40
1:A:341:ILE:HG22	1:A:341:ILE:O	2.22	0.40
2:B:502:LEU:CB	2:B:515:THR:HA	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:597:LEU:HB3	2:B:599:GLU:OE2	2.21	0.40
1:A:211:ASP:O	1:A:215:LYS: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	364/374 (97%)	321 (88%)	33 (9%)	10 (3%)	5	31
2	B	227/231 (98%)	220 (97%)	7 (3%)	0	100	100
All	All	591/605 (98%)	541 (92%)	40 (7%)	10 (2%)	13	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	203	THR
1	A	233	SER
1	A	355	MET
1	A	5	ILE
1	A	40	HIS
1	A	234	SER
1	A	244	ASP
1	A	369	ILE
1	A	46	GLY

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	317/317 (100%)	280 (88%)	37 (12%)	5	21
2	B	212/213 (100%)	207 (98%)	5 (2%)	49	69
All	All	529/530 (100%)	487 (92%)	42 (8%)	16	35

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	34	ILE
1	A	38	PRO
1	A	41	GLN
1	A	59	GLN
1	A	62	ARG
1	A	66	THR
1	A	80	ASP
1	A	93	GLU
1	A	96	VAL
1	A	148	THR
1	A	149	THR
1	A	177	ARG
1	A	178	LEU
1	A	180	LEU
1	A	196	ARG
1	A	203	THR
1	A	206	ARG
1	A	207	GLU
1	A	208	ILE
1	A	210	ARG
1	A	234	SER
1	A	236	LEU
1	A	244	ASP
1	A	246	GLN
1	A	247	VAL
1	A	265	SER
1	A	291	LYS
1	A	324	THR
1	A	335	ARG
1	A	336	LYS
1	A	346	LEU
1	A	350	SER

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Mol	Chain	Res	Type
1	A	360	GLN
1	A	365	SER
1	A	368	SER
1	A	370	VAL
2	B	437	ASN
2	B	563	ASN
2	B	577	ARG
2	B	605	ASN
2	B	612	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	87	HIS
1	A	353	GLN
2	B	403	ASN
2	B	437	ASN
2	B	440	HIS
2	B	457	ASN
2	B	458	GLN
2	B	465	GLN
2	B	492	GLN
2	B	563	ASN
2	B	605	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 monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	335:ARG	C	336:LYS	N	7.03
1	A	145:SER	C	146:GLY	N	6.11
1	B	507:SER	C	513:GLU	N	5.94
1	A	69:TYR	C	70:PRO	N	5.40
1	A	33:SER	C	34:ILE	N	2.67