



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Nov 29, 2017 – 08:22 PM EST

PDB ID : 6B7Y
EMDB ID: : EMD-7065
Title : Cryo-EM structure of human insulin degrading enzyme
Authors : Liang, W.G.; Zhang, Z.; Bailey, L.J.; Kossiakoff, A.A.; Tan, Y.Z.; Wei, H.;
Carragher, B.; Potter, S.C.; Tang, W.J.
Deposited on : unknown
Resolution : 6.50 Å(reported)

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-20030345

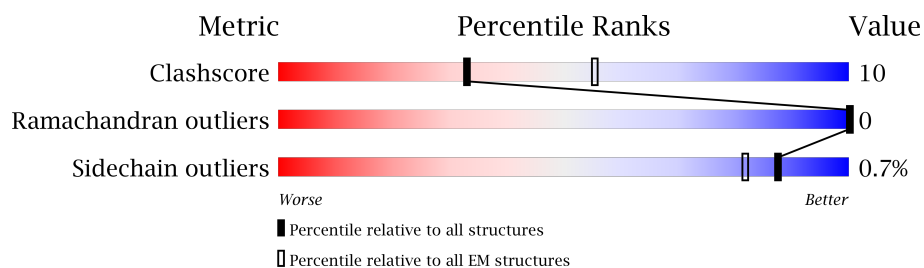
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 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	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	966	
1	B	966	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15410 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	949	Total	C	N	O	S	0	0
			7748	4995	1302	1429	22		
1	B	939	Total	C	N	O	S	0	0
			7662	4942	1284	1415	21		

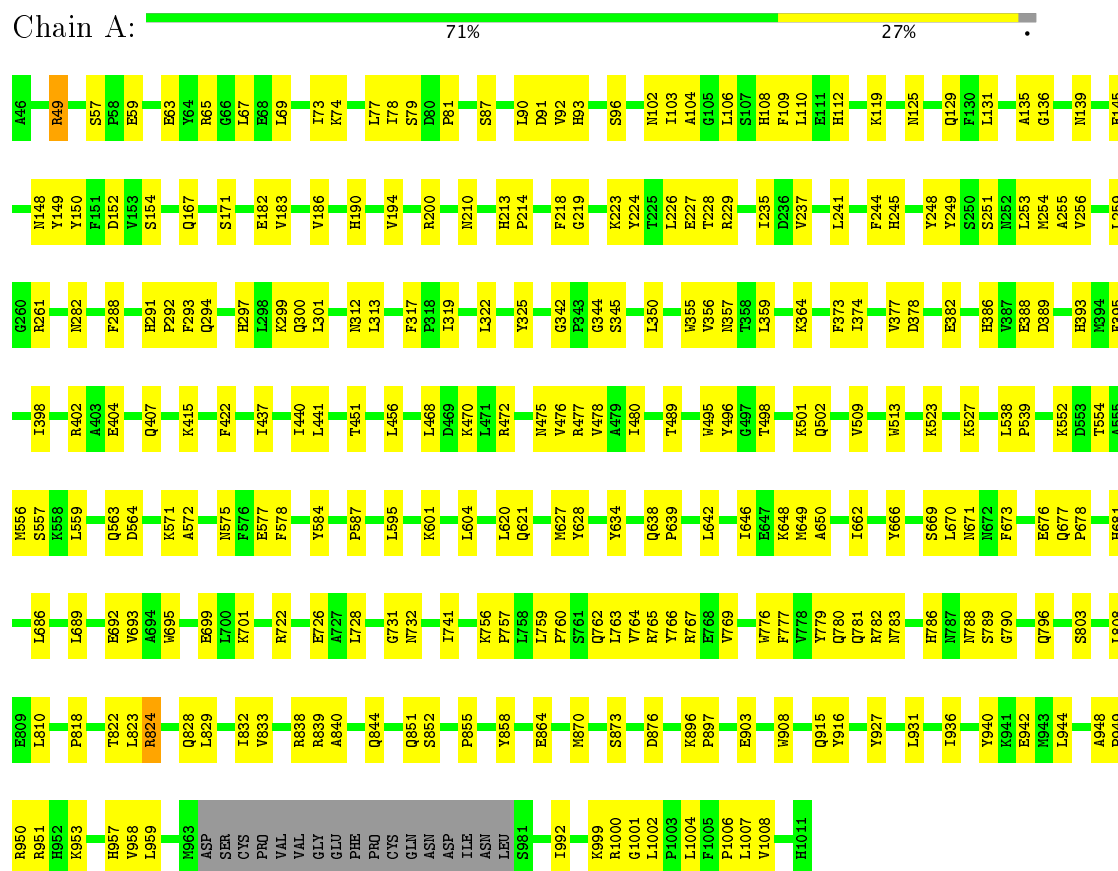
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	CYS	conflict	UNP P14735
A	171	SER	CYS	conflict	UNP P14735
A	178	ALA	CYS	conflict	UNP P14735
A	257	VAL	CYS	conflict	UNP P14735
A	414	LEU	CYS	conflict	UNP P14735
A	573	ASN	CYS	conflict	UNP P14735
A	590	SER	CYS	conflict	UNP P14735
A	789	SER	CYS	conflict	UNP P14735
A	812	ALA	CYS	conflict	UNP P14735
A	819	ALA	CYS	conflict	UNP P14735
A	904	SER	CYS	conflict	UNP P14735
B	110	LEU	CYS	conflict	UNP P14735
B	171	SER	CYS	conflict	UNP P14735
B	178	ALA	CYS	conflict	UNP P14735
B	257	VAL	CYS	conflict	UNP P14735
B	414	LEU	CYS	conflict	UNP P14735
B	573	ASN	CYS	conflict	UNP P14735
B	590	SER	CYS	conflict	UNP P14735
B	789	SER	CYS	conflict	UNP P14735
B	812	ALA	CYS	conflict	UNP P14735
B	819	ALA	CYS	conflict	UNP P14735
B	904	SER	CYS	conflict	UNP P14735

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 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: Insulin-degrading enzyme



• Molecule 1: Insulin-degrading enzyme



V958	F834	V707	F568	V449
L959	L346	R711	K571	L450
E962	I349	L712	A572	E457
MET	I350	H724	N573	E458
ASP	Q851	L725	L574	
SER		E726	N575	P461
CYS	P855	A727	F576	
PRO	P856	L728	E577	I464
VAL	H357		F578	
GLY	Y358	G731	F579	L468
GLU		N732		D469
PHE	F866		D586	
PRO		Q743	P587	R472
CYS	M370		L588	P473
GLN		E746	H589	E474
ASN	S373	D747		N475
ASP		T748	M592	V476
ILE	Q883	L749		R477
ASN	I386		Y596	V478
LEU	Q887	L758	L600	A479
SER	A388	L759	K601	I480
GLN				
ALA	V764		T489	
PRO	R392	R765	L604	
ALA	R393	Y766	M605	I505
LEU	L394			
PRO	D395	W776	A608	E508
GLN	K396		A611	V509
P389	L300	Q780		I510
		R781	L616	Q514
K999	E903	N783	D619	F522
R1000	S904	E784	L620	
G1001	A905		T623	P525
L1002	K906	N788	G625	
P1003		S789	Y626	F530
L1004	F918	G790	M627	
	V925		Y628	I537
L1007	A926	Y795	L629	L538
	Y927	D798	S630	
			G633	Y547
	L931	S803	Y634	P546
	E934	E804		A549
		L810	Q638	L550
	I937			I551
	Y940	I815	L642	K552
				D553
	M943	T822		T554
	L944	L823	M649	S557
		R824	P678	K558
	R950	T825		L559
		K826	E592	I560
	K953	E827		F561
	H957	I832	D706	K562
		W833		Q563
				D564

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24425	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	7.9, 6.8	Depositor
Minimum defocus (nm)	940	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	46598	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor

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 >2	RMSZ	# Z >2
1	A	0.39	0/7942	0.65	0/10744
1	B	0.39	0/7853	0.64	0/10620
All	All	0.39	0/15795	0.65	0/21364

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7748	0	7686	165	0
1	B	7662	0	7581	163	0
All	All	15410	0	15267	321	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 10.

All (321) 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:B:244:PHE:O	1:B:248:TYR:HB2	1.84	0.78
1:B:419:ALA:O	1:B:423:ARG:HB2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ARG:HG2	1:A:844:GLN:HA	1.71	0.71
1:B:245:HIS:HA	1:B:249:TYR:HB2	1.72	0.70
1:A:317:PHE:HB2	1:A:373:PHE:HB3	1.73	0.69
1:B:150:TYR:HB3	1:B:435:SER:HB3	1.73	0.69
1:A:437:ILE:O	1:A:441:LEU:HB2	1.91	0.69
1:B:314:TYR:HB2	1:B:479:ALA:HB3	1.74	0.69
1:A:897:PRO:HG2	1:A:903:GLU:HB3	1.75	0.69
1:B:782:ARG:HA	1:B:959:LEU:HB2	1.75	0.68
1:B:822:THR:O	1:B:826:LYS:HB3	1.93	0.68
1:A:1000:ARG:HH12	1:B:764:VAL:HA	1.59	0.68
1:B:317:PHE:HB2	1:B:373:PHE:HB3	1.76	0.67
1:B:623:THR:HB	1:B:626:GLY:H	1.60	0.67
1:B:834:PHE:HB3	1:B:849:ILE:HB	1.76	0.67
1:B:855:PRO:HB2	1:B:858:TYR:HB3	1.76	0.66
1:B:269:ASN:O	1:B:273:LYS:HB3	1.95	0.66
1:A:838:ARG:HH12	1:A:840:ALA:HB2	1.61	0.65
1:B:823:LEU:HD21	1:B:866:PHE:HB2	1.79	0.65
1:B:346:LEU:HD11	1:B:393:HIS:HB3	1.77	0.65
1:B:795:TYR:HB2	1:B:846:LEU:HB3	1.78	0.65
1:A:78:ILE:HB	1:A:259:LEU:HA	1.79	0.65
1:B:576:PHE:HB2	1:B:629:LEU:HB3	1.80	0.64
1:B:92:VAL:HG22	1:B:254:MET:HG3	1.80	0.63
1:A:782:ARG:HA	1:A:959:LEU:HB2	1.80	0.63
1:B:586:ASP:HB2	1:B:589:HIS:H	1.62	0.63
1:B:578:PHE:HB2	1:B:627:MET:HB2	1.79	0.63
1:A:382:GLU:O	1:A:386:HIS:ND1	2.30	0.63
1:A:103:ILE:HG23	1:A:226:LEU:HA	1.81	0.63
1:A:395:PHE:HE2	1:A:513:TRP:HB3	1.64	0.62
1:B:266:ASP:O	1:B:270:LEU:HB2	2.00	0.62
1:A:74:LYS:HB2	1:A:255:ALA:HA	1.81	0.62
1:B:788:ASN:HB2	1:B:851:GLN:HE21	1.65	0.62
1:B:125:ASN:O	1:B:129:GLN:N	2.32	0.61
1:A:1001:GLY:HA2	1:B:1007:LEU:H	1.65	0.61
1:B:409:TRP:O	1:B:413:GLU:HB2	2.01	0.61
1:A:415:LYS:HG3	1:A:456:LEU:HB2	1.82	0.61
1:B:363:GLN:NE2	1:B:371:MET:SD	2.74	0.60
1:A:109:PHE:HB2	1:A:226:LEU:HD11	1.81	0.60
1:B:293:PHE:HB2	1:B:318:PRO:HG3	1.84	0.60
1:A:621:GLN:O	1:A:628:TYR:N	2.32	0.60
1:A:93:HIS:HB3	1:A:253:LEU:HB3	1.84	0.60
1:B:260:GLY:HA3	1:B:267:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLN:HB3	1:A:502:GLN:HE22	1.67	0.60
1:A:678:PRO:HG3	1:A:783:ASN:HD22	1.67	0.60
1:B:248:TYR:HA	1:B:283:VAL:HG21	1.82	0.59
1:A:1006:PRO:HG3	1:B:1003:PRO:HG3	1.84	0.59
1:B:322:LEU:HD13	1:B:330:PRO:HD2	1.84	0.59
1:B:316:THR:HB	1:B:477:ARG:HB2	1.83	0.59
1:A:646:ILE:O	1:A:650:ALA:HB2	2.03	0.59
1:A:312:ASN:ND2	1:A:377:VAL:O	2.34	0.58
1:B:253:LEU:HD21	1:B:285:LEU:HG	1.84	0.58
1:B:571:LYS:HA	1:B:634:TYR:HA	1.85	0.58
1:B:579:PHE:HB3	1:B:724:HIS:HB3	1.84	0.58
1:A:759:LEU:H	1:A:762:GLN:HE21	1.51	0.58
1:A:538:LEU:O	1:A:563:GLN:NE2	2.36	0.58
1:A:942:GLU:HG3	1:A:950:ARG:HD3	1.86	0.58
1:B:538:LEU:H	1:B:732:ASN:HB3	1.68	0.58
1:A:200:ARG:HD3	1:A:498:THR:HB	1.86	0.57
1:A:190:HIS:HE1	1:A:495:TRP:HB3	1.68	0.57
1:A:790:GLY:N	1:A:958:VAL:O	2.35	0.57
1:B:894:LEU:HD11	1:B:925:VAL:HG11	1.85	0.57
1:A:92:VAL:HG22	1:A:254:MET:HG3	1.87	0.57
1:B:127:TYR:HA	1:B:164:ARG:HD3	1.86	0.57
1:A:575:ASN:HB2	1:A:728:LEU:HB3	1.86	0.57
1:A:489:THR:HA	1:A:501:LYS:HG2	1.86	0.57
1:A:108:HIS:HD2	1:A:186:VAL:HG13	1.69	0.57
1:B:69:LEU:HD21	1:B:272:VAL:HG22	1.87	0.57
1:A:87:SER:HA	1:A:152:ASP:HA	1.87	0.56
1:A:102:ASN:HD22	1:A:235:ILE:HD13	1.70	0.56
1:A:587:PRO:HG3	1:A:695:TRP:HB3	1.86	0.56
1:A:692:GLU:HB2	1:A:766:TYR:HB3	1.88	0.56
1:B:126:GLU:HG3	1:B:164:ARG:HE	1.69	0.56
1:B:327:LYS:HB3	1:B:458:GLU:H	1.70	0.56
1:A:364:LYS:HB2	1:A:374:ILE:HG12	1.88	0.56
1:B:389:ASP:O	1:B:393:HIS:ND1	2.35	0.56
1:B:575:ASN:HB2	1:B:728:LEU:HB3	1.88	0.55
1:A:873:SER:HA	1:A:876:ASP:HB2	1.88	0.55
1:B:63:GLU:HB2	1:B:79:SER:HB3	1.87	0.55
1:B:823:LEU:O	1:B:827:GLU:HB2	2.05	0.55
1:B:87:SER:HB2	1:B:259:LEU:HB3	1.88	0.55
1:B:402:ARG:HG3	1:B:468:LEU:HD21	1.89	0.55
1:B:692:GLU:HB3	1:B:766:TYR:HD1	1.72	0.55
1:A:402:ARG:HA	1:A:468:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:943:MET:HA	1:B:950:ARG:HB2	1.88	0.55
1:A:389:ASP:O	1:A:393:HIS:ND1	2.38	0.55
1:B:303:LYS:HE3	1:B:489:THR:HG22	1.87	0.55
1:B:62:ARG:NH1	1:B:428:GLU:OE2	2.40	0.55
1:A:764:VAL:HA	1:B:1000:ARG:HH12	1.72	0.55
1:A:948:ALA:HB3	1:A:951:ARG:HB2	1.89	0.55
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.89	0.55
1:A:781:GLN:O	1:A:959:LEU:N	2.29	0.54
1:B:91:ASP:HB3	1:B:255:ALA:HB3	1.89	0.54
1:B:575:ASN:HD22	1:B:728:LEU:HD23	1.73	0.54
1:B:69:LEU:HB2	1:B:73:ILE:HB	1.89	0.54
1:B:562:LYS:NZ	1:B:563:GLN:O	2.35	0.54
1:B:575:ASN:ND2	1:B:904:SER:OG	2.40	0.54
1:A:245:HIS:O	1:A:249:TYR:HB2	2.08	0.54
1:A:765:ARG:HB2	1:A:1007:LEU:HD21	1.88	0.54
1:B:776:TRP:CD1	1:B:953:LYS:HG2	2.43	0.54
1:B:299:LYS:NZ	1:B:474:GLU:O	2.39	0.53
1:B:187:ASP:HB2	1:B:223:LYS:HB2	1.89	0.53
1:A:91:ASP:O	1:A:255:ALA:N	2.38	0.53
1:A:572:ALA:HB3	1:A:638:GLN:HE22	1.73	0.53
1:A:595:LEU:HD22	1:A:662:ILE:HG22	1.91	0.53
1:B:382:GLU:O	1:B:386:HIS:ND1	2.31	0.53
1:A:638:GLN:O	1:A:642:LEU:HB3	2.08	0.53
1:A:677:GLN:OE1	1:A:786:HIS:NE2	2.42	0.53
1:A:999:LYS:HA	1:A:1002:LEU:HD12	1.91	0.52
1:B:322:LEU:HD22	1:B:330:PRO:HG2	1.91	0.52
1:A:538:LEU:HD22	1:A:539:PRO:HD2	1.91	0.52
1:B:134:HIS:HB3	1:B:154:SER:H	1.74	0.52
1:A:104:ALA:HB1	1:A:218:PHE:HB3	1.90	0.52
1:A:578:PHE:HD2	1:A:627:MET:HB2	1.75	0.52
1:A:808:LEU:HD12	1:A:839:ARG:HH21	1.75	0.52
1:A:344:GLY:HA3	1:A:523:LYS:H	1.75	0.52
1:B:264:LEU:O	1:B:268:THR:OG1	2.25	0.52
1:A:299:LYS:N	1:A:476:VAL:O	2.40	0.52
1:B:91:ASP:HA	1:B:148:ASN:HA	1.92	0.52
1:B:999:LYS:HA	1:B:1002:LEU:HD12	1.91	0.52
1:A:357:ASN:HB2	1:A:378:ASP:HB3	1.91	0.52
1:B:508:GLU:HG3	1:B:509:VAL:HG23	1.92	0.52
1:A:769:VAL:O	1:A:796:GLN:NE2	2.40	0.51
1:B:71:ASN:ND2	1:B:276:SER:O	2.43	0.51
1:B:780:GLN:HA	1:B:957:HIS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:HG22	1:A:470:LYS:HG2	1.93	0.51
1:A:49:ARG:HB2	1:A:67:LEU:HD22	1.91	0.51
1:B:547:TYR:CG	1:B:918:PHE:HB3	2.46	0.51
1:A:297:HIS:HB3	1:A:477:ARG:HH11	1.76	0.51
1:A:638:GLN:O	1:A:642:LEU:CB	2.59	0.51
1:B:268:THR:O	1:B:272:VAL:HB	2.11	0.51
1:A:119:LYS:HE2	1:A:167:GLN:HE22	1.77	0.50
1:A:789:SER:N	1:A:852:SER:O	2.37	0.50
1:B:832:ILE:HB	1:B:851:GLN:HB3	1.92	0.50
1:B:269:ASN:O	1:B:273:LYS:CB	2.60	0.50
1:B:301:LEU:HA	1:B:478:VAL:HB	1.94	0.50
1:A:673:PHE:HA	1:A:676:GLU:HG2	1.93	0.50
1:A:96:SER:HB2	1:A:219:GLY:HA2	1.94	0.50
1:A:760:PRO:HA	1:A:763:LEU:HB3	1.93	0.50
1:A:190:HIS:CE1	1:A:495:TRP:HB3	2.47	0.49
1:A:686:LEU:HD11	1:A:838:ARG:HG2	1.93	0.49
1:B:400:LYS:HG3	1:B:522:PHE:HB2	1.93	0.49
1:A:824:ARG:HB2	1:A:833:VAL:HG21	1.92	0.49
1:B:73:ILE:HD11	1:B:278:VAL:HB	1.93	0.49
1:B:473:PRO:HG2	1:B:514:GLN:HA	1.94	0.49
1:B:299:LYS:N	1:B:476:VAL:O	2.43	0.49
1:A:131:LEU:O	1:A:136:GLY:N	2.41	0.49
1:A:722:ARG:HG3	1:A:756:LYS:HB2	1.95	0.49
1:B:131:LEU:O	1:B:136:GLY:N	2.45	0.49
1:A:823:LEU:O	1:A:828:GLN:N	2.46	0.49
1:B:592:MET:HB3	1:B:712:LEU:HD13	1.95	0.49
1:B:619:ASP:HB3	1:B:630:SER:HB3	1.93	0.49
1:B:601:LYS:HD2	1:B:620:LEU:HB2	1.95	0.49
1:A:388:GLU:HG2	1:A:509:VAL:HG11	1.94	0.49
1:B:449:VAL:HG23	1:B:450:LEU:HG	1.95	0.49
1:B:810:LEU:HD23	1:B:931:LEU:HD22	1.95	0.49
1:B:943:MET:HG2	1:B:950:ARG:HD2	1.95	0.49
1:A:571:LYS:HA	1:A:634:TYR:HA	1.94	0.48
1:B:469:ASP:HA	1:B:472:ARG:HE	1.77	0.48
1:A:646:ILE:O	1:A:650:ALA:CB	2.61	0.48
1:A:832:ILE:HB	1:A:851:GLN:H	1.78	0.48
1:B:400:LYS:HE3	1:B:522:PHE:HB2	1.95	0.48
1:A:244:PHE:O	1:A:248:TYR:HB2	2.13	0.48
1:B:623:THR:HG22	1:B:625:TYR:H	1.79	0.48
1:A:404:GLU:OE1	1:A:407:GLN:NE2	2.46	0.48
1:A:940:TYR:HA	1:A:944:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:PHE:N	1:B:849:ILE:O	2.41	0.48
1:A:73:ILE:HA	1:A:254:MET:HB2	1.96	0.48
1:B:461:PRO:HA	1:B:464:ILE:HD12	1.95	0.48
1:B:63:GLU:N	1:B:79:SER:O	2.36	0.48
1:B:934:GLU:HA	1:B:937:ILE:HD12	1.95	0.48
1:A:1007:LEU:H	1:B:1001:GLY:HA2	1.78	0.48
1:B:315:VAL:HB	1:B:375:ILE:HB	1.94	0.47
1:B:505:ILE:HB	1:B:510:ILE:HD11	1.96	0.47
1:A:342:GLY:H	1:A:345:SER:HB2	1.77	0.47
1:A:829:LEU:O	1:A:852:SER:OG	2.27	0.47
1:A:210:ASN:HB3	1:A:213:HIS:HB2	1.95	0.47
1:A:639:PRO:HG3	1:A:741:ILE:HD11	1.95	0.47
1:B:573:ASN:HB2	1:B:900:LEU:HD22	1.96	0.47
1:A:317:PHE:HD1	1:A:475:ASN:HB3	1.80	0.47
1:B:798:ASP:HB3	1:B:804:GLU:HG3	1.97	0.47
1:B:596:TYR:O	1:B:600:LEU:HB2	2.14	0.47
1:A:103:ILE:HG21	1:A:106:LEU:HD13	1.96	0.47
1:A:395:PHE:HD1	1:A:398:ILE:HD12	1.80	0.47
1:B:706:ASP:O	1:B:711:ARG:NE	2.47	0.47
1:B:91:ASP:O	1:B:255:ALA:N	2.42	0.47
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.96	0.47
1:B:746:GLU:HA	1:B:749:LEU:HD12	1.97	0.47
1:B:76:LEU:HD23	1:B:437:ILE:HD13	1.96	0.47
1:A:224:TYR:HA	1:A:228:THR:HB	1.97	0.46
1:B:103:ILE:HG12	1:B:230:PRO:HG3	1.97	0.46
1:B:271:VAL:O	1:B:275:PHE:HB2	2.15	0.46
1:B:795:TYR:O	1:B:846:LEU:N	2.48	0.46
1:A:119:LYS:N	1:A:171:SER:OG	2.42	0.46
1:A:210:ASN:N	1:A:292:PRO:O	2.49	0.46
1:A:572:ALA:HA	1:A:731:GLY:HA3	1.97	0.46
1:B:419:ALA:O	1:B:423:ARG:CB	2.60	0.46
1:A:65:ARG:HB3	1:A:77:LEU:HB2	1.96	0.46
1:A:855:PRO:HB2	1:A:858:TYR:HB3	1.97	0.46
1:B:552:LYS:O	1:B:559:LEU:N	2.46	0.46
1:A:139:ASN:HB3	1:A:150:TYR:CZ	2.50	0.46
1:A:87:SER:O	1:A:259:LEU:N	2.49	0.46
1:A:291:HIS:HD2	1:A:293:PHE:HB2	1.81	0.46
1:A:251:SER:HB2	1:A:282:ASN:H	1.81	0.46
1:A:575:ASN:HD22	1:A:728:LEU:HD23	1.80	0.46
1:B:87:SER:HA	1:B:152:ASP:HA	1.97	0.46
1:B:743:GLN:O	1:B:747:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:SER:HA	1:B:927:TYR:CE2	2.51	0.46
1:A:69:LEU:HB2	1:A:73:ILE:HB	1.96	0.46
1:A:81:PRO:HA	1:A:261:ARG:HB2	1.97	0.45
1:B:131:LEU:HD22	1:B:136:GLY:HA3	1.97	0.45
1:B:115:PHE:HE1	1:B:149:TYR:HE1	1.65	0.45
1:A:673:PHE:HZ	1:A:681:HIS:HA	1.81	0.45
1:A:788:ASN:HB2	1:A:851:GLN:HE21	1.80	0.45
1:B:855:PRO:HA	1:B:856:PRO:HD3	1.84	0.45
1:A:322:LEU:HB2	1:A:325:TYR:HB2	1.97	0.45
1:B:205:GLU:OE1	1:B:364:LYS:NZ	2.49	0.45
1:A:1004:LEU:HD12	1:B:1004:LEU:HB2	1.99	0.45
1:B:623:THR:N	1:B:626:GLY:O	2.43	0.45
1:B:251:SER:HB3	1:B:281:LYS:HB2	1.99	0.45
1:B:558:LYS:HD3	1:B:560:TRP:HE1	1.82	0.45
1:B:225:THR:HA	1:B:229:ARG:HD3	1.98	0.45
1:A:915:GLN:HE22	1:A:1008:VAL:HG11	1.82	0.45
1:A:350:LEU:HD13	1:A:356:VAL:HG21	1.98	0.45
1:A:359:LEU:HA	1:A:377:VAL:HA	1.98	0.45
1:B:588:LEU:HD21	1:B:707:VAL:HG22	1.98	0.45
1:B:409:TRP:O	1:B:413:GLU:CB	2.65	0.45
1:B:616:LEU:HG	1:B:633:GLY:HA3	1.99	0.45
1:A:554:THR:HB	1:A:557:SER:H	1.82	0.45
1:B:154:SER:HB3	1:B:157:HIS:CE1	2.51	0.45
1:A:422:PHE:HE2	1:A:451:THR:HG22	1.82	0.44
1:A:601:LYS:HD2	1:A:620:LEU:HB2	1.98	0.44
1:B:815:ILE:HA	1:B:870:MET:HE2	1.99	0.44
1:A:112:HIS:ND1	1:A:182:GLU:OE2	2.50	0.44
1:B:558:LYS:O	1:B:727:ALA:N	2.50	0.44
1:B:870:MET:HA	1:B:873:SER:HB3	1.98	0.44
1:B:604:LEU:O	1:B:608:ALA:N	2.50	0.44
1:A:621:GLN:HB3	1:A:628:TYR:HB3	2.00	0.44
1:A:780:GLN:HA	1:A:957:HIS:HB2	1.99	0.44
1:B:548:PRO:HA	1:B:562:LYS:HB2	1.99	0.44
1:B:564:ASP:HB2	1:B:731:GLY:HA2	1.98	0.44
1:A:87:SER:HB3	1:A:259:LEU:HB3	1.99	0.44
1:A:726:GLU:OE2	1:A:916:TYR:OH	2.35	0.44
1:A:183:VAL:HG22	1:A:223:LYS:HA	1.99	0.43
1:B:178:ALA:O	1:B:182:GLU:HB2	2.18	0.43
1:B:790:GLY:N	1:B:958:VAL:O	2.35	0.43
1:A:301:LEU:HA	1:A:478:VAL:HB	2.00	0.43
1:A:131:LEU:HB3	1:A:136:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:HA	1:A:496:TYR:HD1	1.83	0.43
1:A:556:MET:HB2	1:A:757:PRO:HG3	1.99	0.43
1:A:777:PHE:HB3	1:A:992:ILE:HD11	2.00	0.43
1:A:864:GLU:OE2	1:A:953:LYS:NZ	2.51	0.43
1:A:110:LEU:HD21	1:A:241:LEU:HD22	1.99	0.43
1:A:575:ASN:OD1	1:A:628:TYR:OH	2.36	0.43
1:A:90:LEU:O	1:A:149:TYR:N	2.42	0.43
1:A:63:GLU:HB2	1:A:79:SER:HB3	2.00	0.43
1:A:604:LEU:HD22	1:A:648:LYS:HG2	2.00	0.43
1:A:818:PRO:O	1:A:822:THR:OG1	2.24	0.43
1:A:810:LEU:HD23	1:A:931:LEU:HD22	2.01	0.43
1:A:769:VAL:HA	1:A:1004:LEU:HD23	2.00	0.43
1:B:109:PHE:HZ	1:B:179:LYS:HG3	1.84	0.43
1:B:888:ALA:O	1:B:892:ARG:HB2	2.19	0.43
1:A:671:ASN:HB3	1:A:701:LYS:HD2	2.01	0.42
1:B:301:LEU:HD21	1:B:480:ILE:HD12	2.00	0.42
1:B:327:LYS:HG2	1:B:457:GLU:HB2	2.00	0.42
1:A:227:GLU:HG2	1:A:237:VAL:HG21	2.00	0.42
1:A:803:SER:HA	1:A:927:TYR:CE2	2.54	0.42
1:A:942:GLU:HA	1:A:949:PRO:HD2	2.01	0.42
1:B:364:LYS:HB3	1:B:372:PHE:HB2	2.01	0.42
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.86	0.42
1:A:699:GLU:HG3	1:B:759:LEU:HD21	2.00	0.42
1:A:214:PRO:HB2	1:A:288:PHE:CE1	2.53	0.42
1:A:152:ASP:N	1:A:152:ASP:OD1	2.53	0.42
1:A:402:ARG:NH2	1:A:472:ARG:HH12	2.18	0.42
1:A:91:ASP:HA	1:A:148:ASN:HA	2.02	0.42
1:B:554:THR:OG1	1:B:557:SER:N	2.44	0.42
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.91	0.42
1:B:202:PHE:O	1:B:206:LYS:HG2	2.20	0.42
1:B:110:LEU:HD13	1:B:244:PHE:HD2	1.85	0.42
1:B:883:GLN:HA	1:B:886:ILE:HG12	2.02	0.42
1:A:74:LYS:O	1:A:256:VAL:N	2.43	0.41
1:B:110:LEU:O	1:B:114:LEU:N	2.51	0.41
1:B:210:ASN:N	1:B:292:PRO:O	2.47	0.41
1:A:135:ALA:HB3	1:A:154:SER:HA	2.02	0.41
1:A:776:TRP:CD1	1:A:953:LYS:HG2	2.55	0.41
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.93	0.41
1:A:125:ASN:O	1:A:129:GLN:N	2.36	0.41
1:B:291:HIS:HA	1:B:292:PRO:HD3	1.83	0.41
1:B:724:HIS:HB2	1:B:758:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:ASN:OD1	1:B:784:GLU:N	2.53	0.41
1:A:564:ASP:N	1:A:564:ASP:OD1	2.53	0.41
1:B:578:PHE:HE1	1:B:725:ILE:HG23	1.86	0.41
1:B:93:HIS:HB3	1:B:253:LEU:HB3	2.01	0.41
1:B:537:ILE:HD12	1:B:568:PHE:HB3	2.02	0.41
1:B:574:LEU:HB3	1:B:576:PHE:CE2	2.56	0.41
1:B:605:ASN:HA	1:B:608:ALA:HB3	2.03	0.41
1:A:210:ASN:ND2	1:A:294:GLN:OE1	2.53	0.41
1:A:666:TYR:HA	1:A:669:SER:HB3	2.01	0.41
1:A:93:HIS:CE1	1:A:145:GLU:HB3	2.55	0.41
1:B:903:GLU:HA	1:B:906:LYS:HE3	2.02	0.41
1:A:577:GLU:HB2	1:A:908:TRP:HH2	1.85	0.41
1:B:586:ASP:H	1:B:589:HIS:HB2	1.85	0.41
1:A:57:SER:O	1:A:59:GLU:N	2.54	0.41
1:A:870:MET:HA	1:A:873:SER:HB3	2.03	0.41
1:A:936:ILE:HA	1:A:936:ILE:HD12	1.93	0.41
1:B:1004:LEU:HD23	1:B:1004:LEU:HA	1.96	0.41
1:A:767:ARG:HD3	1:A:1004:LEU:HB3	2.02	0.41
1:A:355:TRP:HD1	1:A:382:GLU:HG3	1.86	0.41
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.85	0.41
1:A:313:LEU:HD13	1:A:480:ILE:HG12	2.02	0.40
1:A:689:LEU:HD11	1:A:779:TYR:HE1	1.86	0.40
1:B:340:HIS:CD2	1:B:525:PRO:HG3	2.57	0.40
1:B:940:TYR:HA	1:B:944:LEU:HD12	2.02	0.40
1:A:300:GLN:OE1	1:A:502:GLN:NE2	2.55	0.40
1:A:584:TYR:HH	1:A:693:VAL:H	1.66	0.40
1:B:350:LEU:HD23	1:B:350:LEU:HA	1.94	0.40
1:B:638:GLN:O	1:B:642:LEU:CB	2.69	0.40
1:B:550:LEU:HD11	1:B:553:ASP:HB2	2.03	0.40
1:B:678:PRO:HG3	1:B:783:ASN:ND2	2.37	0.40
1:B:530:PHE:HE2	1:B:611:ALA:HA	1.86	0.40
1:A:440:ILE:HG13	1:A:440:ILE:H	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	945/966 (98%)	906 (96%)	39 (4%)	0	100	100
1	B	933/966 (97%)	902 (97%)	31 (3%)	0	100	100
All	All	1878/1932 (97%)	1808 (96%)	70 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	840/861 (98%)	833 (99%)	7 (1%)	85	92
1	B	828/861 (96%)	824 (100%)	4 (0%)	91	95
All	All	1668/1722 (97%)	1657 (99%)	11 (1%)	87	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	229	ARG
1	A	527	LYS
1	A	649	MET
1	A	732	ASN
1	A	824	ARG
1	A	896	LYS
1	B	56	LYS
1	B	649	MET
1	B	824	ARG
1	B	896	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	A	190	HIS
1	A	232	GLN
1	A	291	HIS
1	A	300	GLN
1	A	502	GLN
1	A	575	ASN
1	A	638	GLN
1	A	681	HIS
1	A	762	GLN
1	A	844	GLN
1	B	844	GLN
1	B	957	HIS

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.