Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 01:31 pm BST

PDB ID	:	1DTE
Title	:	THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE
Authors	:	Brozozowski, A.M.; Savage, H.
Deposited on	:	2000-01-12
Resolution	:	2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

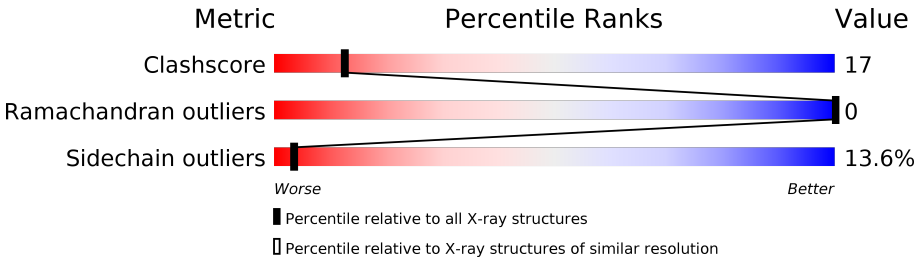
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	57% 31% 9% .
1	B	269	52% 35% 11% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4428 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	9	0	0
			2071	1303	359	403	6			
1	B	269	Total	C	N	O	S	9	0	0
			2071	1303	359	403	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	10	0
			122	122		
2	B	164	Total	O	45	0
			164	164		

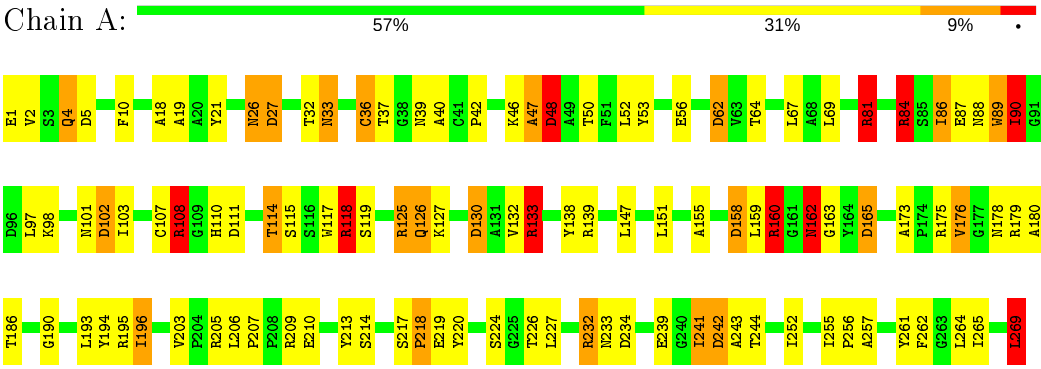
3 Residue-property plots (i)

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

Note EDS was not executed.

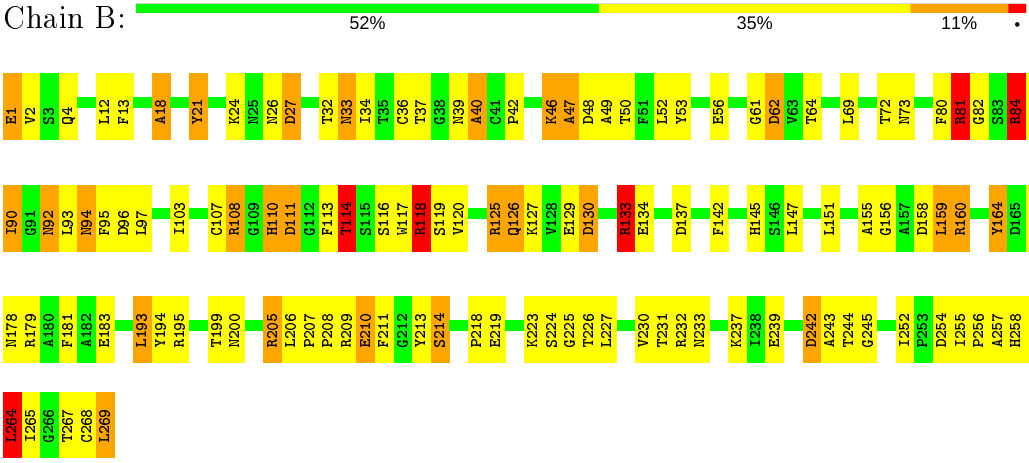
- Molecule 1: LIPASE

Chain A:



- Molecule 1: LIPASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	96.13Å 71.10Å 82.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35	Depositor
% Data completeness (in resolution range)	88.9 (20.00-2.35)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.263 , 0.352	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4428	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.85	1/2121 (0.0%)	2.19	82/2887 (2.8%)
1	B	0.86	2/2121 (0.1%)	2.26	89/2887 (3.1%)
All	All	0.86	3/4242 (0.1%)	2.22	171/5774 (3.0%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	GLU	C-N	10.74	1.58	1.34
1	B	1	GLU	C-N	9.08	1.54	1.34
1	B	245	GLY	N-CA	5.08	1.53	1.46

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	ARG	NE-CZ-NH1	26.58	133.59	120.30
1	B	81	ARG	NE-CZ-NH2	-20.45	110.07	120.30
1	B	195	ARG	NE-CZ-NH1	-19.06	110.77	120.30
1	B	27	ASP	CB-CG-OD2	18.30	134.77	118.30
1	A	175	ARG	NE-CZ-NH1	-15.17	112.71	120.30
1	A	160	ARG	NH1-CZ-NH2	-14.74	103.19	119.40
1	B	175	ARG	NE-CZ-NH2	14.61	127.60	120.30
1	B	160	ARG	CD-NE-CZ	14.37	143.72	123.60
1	B	195	ARG	NE-CZ-NH2	13.73	127.17	120.30
1	B	160	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	A	27	ASP	CB-CG-OD2	13.58	130.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	ARG	NE-CZ-NH2	-13.38	113.61	120.30
1	B	27	ASP	CB-CG-OD1	-12.86	106.72	118.30
1	B	125	ARG	NE-CZ-NH1	12.69	126.64	120.30
1	B	175	ARG	NE-CZ-NH1	-12.62	113.99	120.30
1	A	219	GLU	OE1-CD-OE2	-12.29	108.55	123.30
1	B	195	ARG	CD-NE-CZ	12.14	140.60	123.60
1	B	1	GLU	O-C-N	12.10	142.05	122.70
1	A	130	ASP	CB-CG-OD1	12.01	129.11	118.30
1	A	162	ASN	CA-CB-CG	11.88	139.54	113.40
1	B	244	THR	CA-C-N	11.77	139.73	116.20
1	A	195	ARG	NE-CZ-NH2	11.58	126.09	120.30
1	A	84	ARG	NE-CZ-NH2	11.42	126.01	120.30
1	B	210	GLU	CA-CB-CG	11.41	138.50	113.40
1	A	242	ASP	CB-CG-OD2	11.40	128.56	118.30
1	B	160	ARG	NH1-CZ-NH2	-11.25	107.02	119.40
1	A	160	ARG	CD-NE-CZ	11.21	139.29	123.60
1	B	160	ARG	NE-CZ-NH2	11.12	125.86	120.30
1	B	244	THR	O-C-N	-11.01	104.49	123.20
1	B	254	ASP	CB-CG-OD2	10.97	128.18	118.30
1	B	219	GLU	OE1-CD-OE2	-10.88	110.25	123.30
1	B	84	ARG	NE-CZ-NH1	10.57	125.58	120.30
1	B	1	GLU	CA-C-N	-10.01	95.17	117.20
1	A	244	THR	O-C-N	-9.67	106.76	123.20
1	B	47	ALA	CA-C-N	9.53	138.16	117.20
1	A	27	ASP	CB-CG-OD1	-9.35	109.89	118.30
1	B	21	TYR	CB-CG-CD1	9.28	126.57	121.00
1	B	47	ALA	O-C-N	-9.12	108.10	122.70
1	A	165	ASP	CB-CG-OD1	9.08	126.47	118.30
1	B	126	GLN	CA-CB-CG	9.04	133.30	113.40
1	B	194	TYR	CB-CG-CD2	8.95	126.37	121.00
1	B	205	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	A	118	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	A	47	ALA	CA-C-N	8.84	136.65	117.20
1	B	242	ASP	CB-CG-OD2	8.83	126.24	118.30
1	A	4	GLN	OE1-CD-NE2	-8.76	101.75	121.90
1	A	125	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	B	27	ASP	N-CA-CB	-8.51	95.29	110.60
1	A	210	GLU	CA-CB-CG	8.45	131.98	113.40
1	B	205	ARG	CG-CD-NE	8.45	129.54	111.80
1	A	92	ASN	CB-CG-ND2	8.40	136.86	116.70
1	A	133	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	B	84	ARG	NH1-CZ-NH2	-8.19	110.39	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	81	ARG	NH1-CZ-NH2	8.17	128.39	119.40
1	B	125	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	1	GLU	O-C-N	8.11	135.68	122.70
1	A	84	ARG	NH1-CZ-NH2	-8.07	110.53	119.40
1	A	125	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	B	205	ARG	CD-NE-CZ	-7.89	112.55	123.60
1	B	62	ASP	CB-CG-OD1	7.83	125.35	118.30
1	B	194	TYR	CB-CG-CD1	-7.77	116.34	121.00
1	A	21	TYR	CD1-CG-CD2	-7.76	109.37	117.90
1	B	21	TYR	CD1-CG-CD2	-7.70	109.43	117.90
1	B	242	ASP	OD1-CG-OD2	-7.52	109.01	123.30
1	A	139	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	95	PHE	CB-CG-CD2	-7.42	115.60	120.80
1	A	195	ARG	CD-NE-CZ	7.39	133.95	123.60
1	A	132	VAL	CA-CB-CG1	7.37	121.96	110.90
1	A	244	THR	CA-C-N	7.36	130.91	116.20
1	B	118	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	1	GLU	C-N-CA	-7.24	103.60	121.70
1	A	126	GLN	CA-CB-CG	7.21	129.26	113.40
1	A	220	TYR	CB-CG-CD1	-7.19	116.69	121.00
1	A	21	TYR	CB-CG-CD1	7.18	125.31	121.00
1	B	84	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	B	193	LEU	O-C-N	-7.16	111.25	122.70
1	B	242	ASP	CB-CG-OD1	7.15	124.74	118.30
1	A	118	ARG	NH1-CZ-NH2	7.13	127.24	119.40
1	A	21	TYR	CB-CG-CD2	7.12	125.27	121.00
1	B	1	GLU	C-N-CA	-7.04	104.09	121.70
1	A	1	GLU	CA-C-N	-7.02	101.76	117.20
1	A	218	PRO	N-CA-CB	-6.96	94.94	102.60
1	B	133	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	118	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	A	40	ALA	CB-CA-C	6.82	120.34	110.10
1	A	21	TYR	CG-CD2-CE2	6.80	126.74	121.30
1	A	92	ASN	OD1-CG-ND2	-6.68	106.53	121.90
1	A	47	ALA	O-C-N	-6.63	112.09	122.70
1	B	21	TYR	CG-CD1-CE1	6.55	126.54	121.30
1	A	160	ARG	N-CA-CB	6.51	122.32	110.60
1	A	111	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	209	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	4	GLN	OE1-CD-NE2	-6.36	107.28	121.90
1	A	205	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	B	258	HIS	CA-C-N	6.31	131.09	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	ILE	CB-CA-C	6.29	124.19	111.60
1	A	133	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	B	84	ARG	CD-NE-CZ	6.25	132.35	123.60
1	B	114	THR	N-CA-CB	-6.23	98.47	110.30
1	B	199	THR	CA-CB-CG2	-6.18	103.75	112.40
1	A	36	CYS	CA-CB-SG	6.17	125.10	114.00
1	B	62	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	214	SER	N-CA-CB	-6.11	101.34	110.50
1	B	133	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	5	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	B	40	ALA	CB-CA-C	6.05	119.17	110.10
1	B	219	GLU	CG-CD-OE2	6.02	130.34	118.30
1	A	160	ARG	O-C-N	6.01	133.42	123.20
1	B	92	ASN	OD1-CG-ND2	-6.00	108.11	121.90
1	B	114	THR	O-C-N	-5.99	113.11	122.70
1	B	160	ARG	C-N-CA	-5.96	109.80	122.30
1	A	241	ILE	CB-CG1-CD1	5.92	130.48	113.90
1	A	175	ARG	NH1-CZ-NH2	5.88	125.86	119.40
1	B	110	HIS	CA-CB-CG	5.87	123.58	113.60
1	A	48	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	209	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	232	ARG	CD-NE-CZ	5.86	131.80	123.60
1	A	205	ARG	CD-NE-CZ	-5.83	115.43	123.60
1	B	111	ASP	CA-C-N	5.77	127.74	116.20
1	A	90	ILE	N-CA-CB	-5.76	97.56	110.80
1	A	84	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	160	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	B	225	GLY	C-N-CA	5.70	135.96	121.70
1	B	73	ASN	OD1-CG-ND2	-5.67	108.87	121.90
1	B	233	ASN	OD1-CG-ND2	-5.63	108.96	121.90
1	A	261	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	158	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	261	TYR	CA-CB-CG	-5.57	102.81	113.40
1	B	137	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	88	ASN	O-C-N	-5.51	113.89	122.70
1	A	233	ASN	OD1-CG-ND2	-5.46	109.34	121.90
1	B	27	ASP	CA-CB-CG	5.45	125.39	113.40
1	B	134	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	B	176	VAL	CG1-CB-CG2	5.37	119.49	110.90
1	B	262	PHE	N-CA-CB	5.34	120.22	110.60
1	B	269	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	118	ARG	NH1-CZ-NH2	5.32	125.25	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	210	GLU	CG-CD-OE2	5.32	128.94	118.30
1	A	138	TYR	CB-CG-CD1	5.31	124.19	121.00
1	A	196	ILE	CA-C-O	5.31	131.24	120.10
1	B	18	ALA	CA-C-O	5.30	131.22	120.10
1	B	130	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	163	GLY	N-CA-C	5.28	126.29	113.10
1	A	262	PHE	N-CA-CB	5.28	120.10	110.60
1	A	108	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	115	SER	CA-CB-OG	-5.26	96.99	111.20
1	B	133	ARG	CD-NE-CZ	5.26	130.97	123.60
1	A	95	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	B	80	PHE	CA-C-O	5.25	131.13	120.10
1	B	13	PHE	CB-CA-C	5.22	120.85	110.40
1	B	90	ILE	CB-CA-C	5.22	122.04	111.60
1	A	173	ALA	CB-CA-C	5.18	117.87	110.10
1	A	48	ASP	CA-CB-CG	5.17	124.78	113.40
1	B	113	PHE	CB-CG-CD1	5.17	124.42	120.80
1	B	224	SER	C-N-CA	-5.17	111.45	122.30
1	B	159	LEU	O-C-N	-5.16	114.44	122.70
1	A	269	LEU	CA-CB-CG	5.13	127.10	115.30
1	B	85	SER	CA-C-O	5.12	130.85	120.10
1	A	180	ALA	N-CA-CB	5.12	117.26	110.10
1	A	176	VAL	CG1-CB-CG2	5.09	119.04	110.90
1	B	18	ALA	O-C-N	-5.09	114.56	122.70
1	A	196	ILE	O-C-N	-5.09	114.56	122.70
1	A	21	TYR	CD1-CE1-CZ	5.08	124.37	119.80
1	B	237	LYS	CA-C-O	-5.08	109.44	120.10
1	B	261	TYR	CA-CB-CG	-5.05	103.80	113.40
1	A	176	VAL	N-CA-CB	-5.03	100.43	111.50
1	A	118	ARG	CB-CA-C	-5.03	100.34	110.40
1	A	89	TRP	CA-CB-CG	-5.02	104.17	113.70
1	B	164	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	B	264	LEU	CB-CG-CD1	5.01	119.51	111.00
1	A	81	ARG	NH1-CZ-NH2	5.00	124.90	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	242	ASP	Mainchain

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	2071	0	1965	64	0
1	B	2071	0	1965	70	0
2	A	122	0	0	17	1
2	B	164	0	0	24	2
All	All	4428	0	3930	134	2

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 17.

All (134) 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:259:LEU:HD23	2:B:348:HOH:O	1.70	0.91
1:B:107:CYS:HB3	1:B:181:PHE:HB2	1.58	0.86
1:B:34:ILE:HB	2:B:333:HOH:O	1.76	0.84
1:B:160:ARG:HG3	2:B:374:HOH:O	1.78	0.83
1:A:126:GLN:HG2	2:A:391:HOH:O	1.81	0.80
1:B:114:THR:HG22	2:B:334:HOH:O	1.81	0.80
1:B:166:ILE:HD12	2:B:374:HOH:O	1.81	0.79
1:A:206:LEU:HD12	2:A:310:HOH:O	1.83	0.78
1:A:114:THR:HG22	2:A:313:HOH:O	1.83	0.78
1:A:110:HIS:O	1:A:114:THR:HB	1.84	0.78
1:A:126:GLN:CG	2:A:391:HOH:O	2.33	0.75
1:A:107:CYS:HB3	1:A:181:PHE:HB2	1.70	0.72
1:A:26:ASN:HB2	1:A:56:GLU:HG3	1.71	0.71
1:B:142:PHE:CZ	1:B:166:ILE:HD13	2.26	0.71
1:A:84:ARG:HG3	1:A:84:ARG:HH11	1.56	0.71
1:A:269:LEU:HD22	2:A:320:HOH:O	1.92	0.69
1:A:217:SER:HB3	2:A:324:HOH:O	1.93	0.69
1:A:102:ASP:HB3	2:A:386:HOH:O	1.92	0.68
1:A:232:ARG:HD3	2:A:297:HOH:O	1.94	0.67
1:B:166:ILE:HB	2:B:374:HOH:O	1.93	0.67
1:B:110:HIS:O	1:B:114:THR:HB	1.93	0.66
1:B:12:LEU:HD11	2:B:366:HOH:O	1.94	0.66
1:A:203:VAL:HA	2:A:310:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HB3	2:A:387:HOH:O	2.00	0.60
1:B:166:ILE:CG1	2:B:374:HOH:O	2.49	0.60
1:B:164:TYR:HE2	1:B:166:ILE:HD11	1.66	0.59
1:A:206:LEU:HA	1:A:207:PRO:C	2.23	0.58
1:A:33:ASN:HD22	1:A:33:ASN:N	2.02	0.58
1:B:206:LEU:HA	1:B:207:PRO:C	2.24	0.58
1:A:217:SER:CB	2:A:324:HOH:O	2.49	0.58
1:A:84:ARG:CZ	2:A:275:HOH:O	2.51	0.58
1:B:166:ILE:CB	2:B:374:HOH:O	2.52	0.57
1:B:103:ILE:HD11	1:B:118:ARG:HH12	1.70	0.57
1:B:84:ARG:HG3	1:B:84:ARG:HH11	1.70	0.56
1:B:64:THR:HB	1:B:81:ARG:HD2	1.87	0.56
1:A:32:THR:O	1:A:50:THR:HA	2.05	0.56
1:B:26:ASN:HB2	1:B:56:GLU:HG3	1.88	0.56
1:B:84:ARG:CZ	2:B:287:HOH:O	2.54	0.55
1:A:162:ASN:HB3	2:A:290:HOH:O	2.06	0.55
1:B:243:ALA:HB1	2:B:307:HOH:O	2.06	0.55
1:B:32:THR:O	1:B:50:THR:HA	2.06	0.55
1:B:145:HIS:HE1	2:B:348:HOH:O	1.89	0.54
1:A:27:ASP:HB3	1:A:56:GLU:OE1	2.07	0.54
1:B:207:PRO:HG2	1:B:213:TYR:CZ	2.43	0.54
1:B:33:ASN:N	1:B:33:ASN:HD22	2.06	0.54
1:B:255:ILE:HB	1:B:256:PRO:HD3	1.90	0.54
1:B:42:PRO:O	1:B:46:LYS:HB2	2.07	0.54
1:A:130:ASP:O	1:A:133:ARG:HD2	2.07	0.54
1:B:156:GLY:O	1:B:160:ARG:HD2	2.08	0.54
1:A:255:ILE:HB	1:A:256:PRO:HD3	1.90	0.53
1:A:2:VAL:O	1:A:232:ARG:HB2	2.09	0.53
1:A:39:ASN:OD1	1:A:42:PRO:HG3	2.09	0.52
1:B:118:ARG:NH2	1:B:158:ASP:OD2	2.43	0.52
1:B:232:ARG:HD3	2:B:275:HOH:O	2.08	0.52
1:A:242:ASP:O	1:A:243:ALA:C	2.45	0.52
1:B:268:CYS:HA	2:B:289:HOH:O	2.09	0.52
1:A:64:THR:HB	1:A:81:ARG:HD2	1.92	0.51
1:B:18:ALA:HB2	1:B:265:ILE:HG13	1.92	0.51
1:B:108:ARG:HB2	1:B:178:ASN:ND2	2.26	0.51
1:A:53:TYR:CD1	1:A:127:LYS:HE3	2.46	0.51
1:A:241:ILE:HG13	2:A:324:HOH:O	2.11	0.50
1:A:84:ARG:NH1	2:A:275:HOH:O	2.43	0.50
1:B:94:ASN:ND2	1:B:96:ASP:OD2	2.44	0.50
1:B:53:TYR:CD1	1:B:127:LYS:HE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:VAL:O	1:B:232:ARG:HB2	2.11	0.50
1:B:84:ARG:NH1	2:B:287:HOH:O	2.45	0.50
1:A:84:ARG:HG3	1:A:84:ARG:NH1	2.20	0.50
1:B:226:THR:HG22	1:B:227:LEU:HG	1.93	0.50
1:A:207:PRO:HG2	1:A:213:TYR:CZ	2.47	0.49
1:A:4:GLN:HE21	1:A:232:ARG:HD2	1.77	0.49
1:B:130:ASP:O	1:B:133:ARG:HD2	2.13	0.49
1:A:193:LEU:HD12	1:A:194:TYR:N	2.27	0.49
1:B:62:ASP:CG	2:B:335:HOH:O	2.50	0.49
1:A:52:LEU:HD21	1:A:69:LEU:HB2	1.95	0.48
1:B:27:ASP:HB3	2:B:342:HOH:O	2.12	0.48
1:B:47:ALA:HB1	1:B:72:THR:HB	1.94	0.48
1:A:26:ASN:CB	1:A:56:GLU:HG3	2.43	0.48
1:B:125:ARG:O	1:B:129:GLU:HG3	2.13	0.48
1:A:108:ARG:HB2	1:A:178:ASN:ND2	2.29	0.48
1:B:256:PRO:O	1:B:257:ALA:C	2.52	0.48
1:B:230:VAL:HG12	1:B:231:THR:N	2.28	0.47
1:B:145:HIS:CE1	2:B:348:HOH:O	2.65	0.47
1:A:62:ASP:HB3	1:A:88:ASN:HD21	1.79	0.47
1:B:116:SER:O	1:B:120:VAL:HG22	2.15	0.47
1:B:62:ASP:HB3	1:B:88:ASN:HD21	1.80	0.47
1:A:125:ARG:CD	1:A:159:LEU:HD22	2.46	0.46
1:A:224:SER:HB3	1:A:234:ASP:OD1	2.15	0.46
1:A:265:ILE:HG23	1:A:265:ILE:O	2.16	0.46
1:A:18:ALA:HB2	1:A:265:ILE:HG13	1.97	0.46
1:B:62:ASP:HB3	1:B:88:ASN:ND2	2.30	0.46
1:A:87:GLU:O	1:A:90:ILE:HG22	2.17	0.45
1:A:165:ASP:OD1	1:A:190:GLY:HA2	2.16	0.45
1:A:160:ARG:HG2	1:A:190:GLY:O	2.16	0.45
1:A:86:ILE:O	1:A:90:ILE:HB	2.16	0.45
1:B:164:TYR:CE2	1:B:166:ILE:HD11	2.50	0.45
1:A:89:TRP:HA	1:A:92:ASN:HD22	1.81	0.45
1:A:97:LEU:HB3	1:A:108:ARG:HG2	1.99	0.44
1:B:223:LYS:HD2	2:B:288:HOH:O	2.17	0.44
1:B:84:ARG:HG3	1:B:84:ARG:NH1	2.31	0.44
1:B:84:ARG:NH2	2:B:287:HOH:O	2.50	0.44
1:A:256:PRO:O	1:A:257:ALA:C	2.55	0.44
1:A:117:TRP:CE3	1:A:155:ALA:HB2	2.53	0.44
1:B:92:ASN:O	2:B:364:HOH:O	2.21	0.43
1:A:186:THR:HG23	1:A:217:SER:O	2.19	0.43
1:B:117:TRP:CE3	1:B:155:ALA:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:HA	1:B:151:LEU:HD23	1.86	0.43
1:B:39:ASN:OD1	1:B:42:PRO:HG3	2.18	0.43
1:B:97:LEU:HB3	1:B:108:ARG:HG2	2.00	0.43
1:A:19:ALA:HB2	1:A:36:CYS:SG	2.59	0.43
1:B:34:ILE:HG13	1:B:49:ALA:O	2.19	0.42
1:A:10:PHE:CD1	1:A:196:ILE:HD11	2.53	0.42
1:B:61:GLY:O	1:B:62:ASP:HB2	2.19	0.42
1:B:24:LYS:HA	2:B:342:HOH:O	2.19	0.42
1:A:62:ASP:HB3	1:A:88:ASN:ND2	2.35	0.42
1:B:200:ASN:HB3	2:B:340:HOH:O	2.19	0.42
1:B:52:LEU:HD21	1:B:69:LEU:HB2	2.01	0.42
1:B:125:ARG:CD	1:B:159:LEU:HD22	2.50	0.41
1:B:208:PRO:HG2	1:B:211:PHE:CD1	2.55	0.41
1:A:207:PRO:HG2	1:A:213:TYR:CE1	2.55	0.41
1:A:84:ARG:NH2	2:A:275:HOH:O	2.52	0.41
1:B:36:CYS:HB3	1:B:40:ALA:HB3	2.03	0.41
1:A:47:ALA:O	1:A:48:ASP:HB3	2.21	0.41
1:B:21:TYR:OH	1:B:82:GLY:HA3	2.21	0.41
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.94	0.41
1:A:118:ARG:NH2	1:A:158:ASP:OD2	2.54	0.41
1:B:96:ASP:CG	2:B:318:HOH:O	2.58	0.41
1:A:98:LYS:O	1:A:108:ARG:HA	2.19	0.41
1:A:103:ILE:HD11	1:A:118:ARG:HH12	1.86	0.40
1:B:205:ARG:HD2	1:B:205:ARG:HH11	1.27	0.40
1:A:102:ASP:HA	2:A:386:HOH:O	2.22	0.40
1:A:226:THR:HG22	1:A:227:LEU:HG	2.02	0.40
1:B:260:TRP:HE3	1:B:264:LEU:HD13	1.86	0.40
1:A:67:LEU:CD2	1:A:127:LYS:HB3	2.52	0.40
1:B:94:ASN:ND2	1:B:111:ASP:HB3	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:387:HOH:O	2:B:275:HOH:O[2_664]	2.02	0.18
2:B:300:HOH:O	2:B:329:HOH:O[3_657]	2.14	0.06

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 X-ray entries followed by that with respect to entries of similar resolution.

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	267/269 (99%)	252 (94%)	15 (6%)	0	100	100
1	B	267/269 (99%)	250 (94%)	17 (6%)	0	100	100
All	All	534/538 (99%)	502 (94%)	32 (6%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	220/220 (100%)	190 (86%)	30 (14%)	3	3
1	B	220/220 (100%)	190 (86%)	30 (14%)	3	3
All	All	440/440 (100%)	380 (86%)	60 (14%)	3	3

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	33	ASN
1	A	37	THR
1	A	46	LYS
1	A	48	ASP
1	A	62	ASP
1	A	81	ARG
1	A	84	ARG

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Mol	Chain	Res	Type
1	A	86	ILE
1	A	90	ILE
1	A	93	LEU
1	A	94	ASN
1	A	102	ASP
1	A	108	ARG
1	A	114	THR
1	A	118	ARG
1	A	119	SER
1	A	133	ARG
1	A	147	LEU
1	A	160	ARG
1	A	162	ASN
1	A	176	VAL
1	A	179	ARG
1	A	183	GLU
1	A	214	SER
1	A	218	PRO
1	A	239	GLU
1	A	252	ILE
1	A	264	LEU
1	A	269	LEU
1	B	1	GLU
1	B	33	ASN
1	B	37	THR
1	B	46	LYS
1	B	48	ASP
1	B	81	ARG
1	B	84	ARG
1	B	86	ILE
1	B	90	ILE
1	B	93	LEU
1	B	94	ASN
1	B	108	ARG
1	B	114	THR
1	B	118	ARG
1	B	119	SER
1	B	126	GLN
1	B	133	ARG
1	B	147	LEU
1	B	176	VAL
1	B	179	ARG

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Mol	Chain	Res	Type
1	B	183	GLU
1	B	193	LEU
1	B	210	GLU
1	B	214	SER
1	B	218	PRO
1	B	239	GLU
1	B	252	ILE
1	B	264	LEU
1	B	267	THR
1	B	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	11	ASN
1	A	33	ASN
1	A	92	ASN
1	A	94	ASN
1	B	33	ASN
1	B	73	ASN
1	B	94	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.