Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 02:30 PM EDT

PDB ID	:	1DT3
Title	:	THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE
Authors	:	Brozozowski, A.M.; Savage, H.
Deposited on	:	2000-01-11
Resolution	:	2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

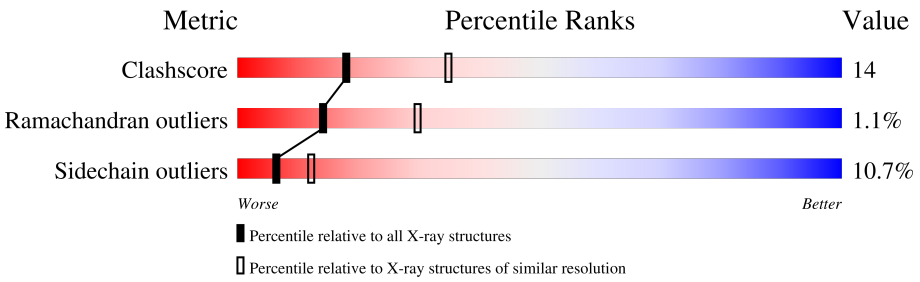
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 of 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% 29% 11% •
1	B	269	55% 32% 10% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4384 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
			Total	C	N	O	S			
1	A	269	2071	1303	359	403	6	0	0	0
1	B	269	2071	1303	359	403	6	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	99	99	99	0	0
2	B	143	143	143	0	0

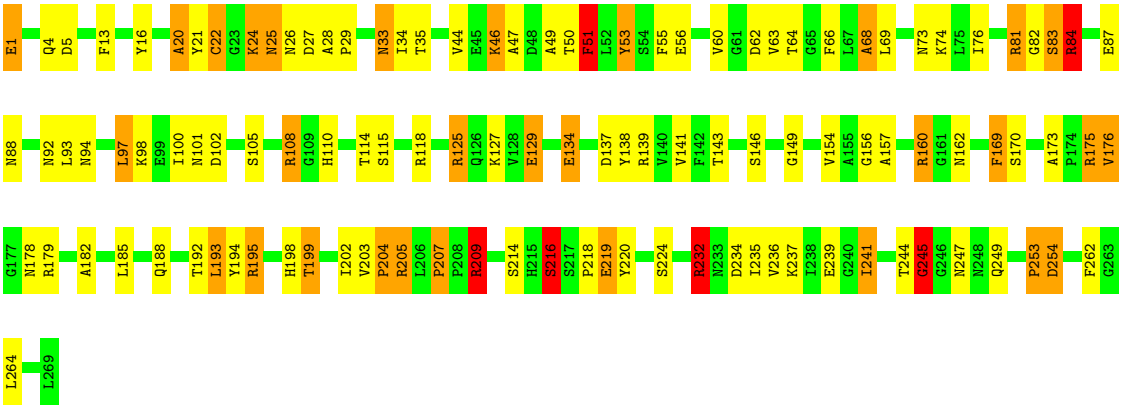
3 Residue-property plots (i)

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.

Note EDS was not executed.

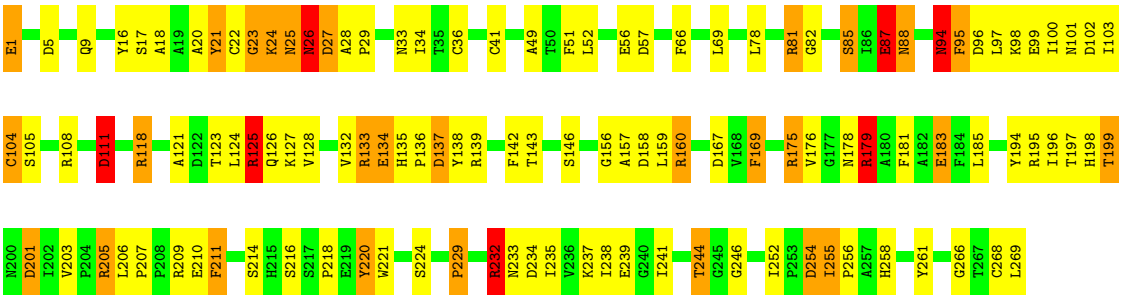
• Molecule 1: LIPASE

Chain A: 57% 29% 11% •



• Molecule 1: LIPASE

Chain B: 55% 32% 10% •



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	139.92Å 139.92Å 80.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.4 (20.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.228 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4384	wwPDB-VP
Average B, all atoms (Å^2)	50.0	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	0.69	1/2121 (0.0%)	1.95	58/2887 (2.0%)
1	B	0.70	0/2121	1.91	53/2887 (1.8%)
All	All	0.69	1/4242 (0.0%)	1.93	111/5774 (1.9%)

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	26
1	B	0	24
All	All	0	50

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	SER	CB-OG	5.73	1.49	1.42

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	195	ARG	CD-NE-CZ	36.84	175.18	123.60
1	A	205	ARG	CD-NE-CZ	21.49	153.69	123.60
1	A	21	TYR	CB-CG-CD2	-15.44	111.74	121.00
1	A	129	GLU	OE1-CD-OE2	15.43	141.82	123.30
1	A	81	ARG	NE-CZ-NH1	15.04	127.82	120.30
1	A	232	ARG	NE-CZ-NH2	-14.96	112.82	120.30
1	A	21	TYR	CB-CG-CD1	12.89	128.73	121.00
1	A	125	ARG	NE-CZ-NH2	12.76	126.68	120.30
1	A	209	ARG	CD-NE-CZ	11.99	140.39	123.60
1	A	195	ARG	NE-CZ-NH1	-11.98	114.31	120.30
1	B	81	ARG	NE-CZ-NH1	11.91	126.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	ARG	NE-CZ-NH2	11.90	126.25	120.30
1	B	118	ARG	NE-CZ-NH1	11.79	126.20	120.30
1	B	138	TYR	CB-CG-CD2	-10.95	114.43	121.00
1	A	245	GLY	C-N-CA	10.53	144.42	122.30
1	A	205	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	A	84	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	B	125	ARG	NE-CZ-NH2	10.27	125.43	120.30
1	B	138	TYR	CB-CG-CD1	9.71	126.83	121.00
1	A	254	ASP	CB-CG-OD1	-9.57	109.69	118.30
1	B	118	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	A	209	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	B	24	LYS	C-N-CA	9.36	145.09	121.70
1	A	108	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	B	133	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	A	139	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	A	232	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	A	84	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	A	160	ARG	NE-CZ-NH1	-8.80	115.90	120.30
1	A	16	TYR	CB-CG-CD2	-8.70	115.78	121.00
1	A	175	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	B	205	ARG	CD-NE-CZ	8.30	135.22	123.60
1	B	104	CYS	N-CA-CB	8.11	125.19	110.60
1	A	125	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	B	111	ASP	CB-CG-OD1	7.82	125.34	118.30
1	A	5	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	B	229	PRO	O-C-N	-7.70	110.38	122.70
1	B	232	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	B	9	GLN	CA-CB-CG	7.21	129.27	113.40
1	A	234	ASP	CB-CG-OD1	-7.20	111.82	118.30
1	A	254	ASP	N-CA-CB	-7.03	97.95	110.60
1	B	88	ASN	CB-CA-C	6.97	124.34	110.40
1	A	22	CYS	CA-C-N	-6.86	102.47	116.20
1	B	205	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	195	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	B	254	ASP	CB-CG-OD2	6.63	124.27	118.30
1	B	138	TYR	C-N-CA	6.51	137.98	121.70
1	A	175	ARG	NH1-CZ-NH2	6.50	126.55	119.40
1	A	219	GLU	OE1-CD-OE2	-6.46	115.55	123.30
1	A	125	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	262	PHE	C-N-CA	6.35	135.64	122.30
1	B	160	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	A	205	ARG	CB-CG-CD	6.18	127.68	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169	PHE	CB-CG-CD2	6.15	125.10	120.80
1	A	134	GLU	O-C-N	-6.11	112.92	122.70
1	A	175	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	26	ASN	CB-CA-C	6.08	122.55	110.40
1	B	24	LYS	O-C-N	-5.92	113.23	122.70
1	B	179	ARG	N-CA-CB	5.83	121.09	110.60
1	B	87	GLU	CA-CB-CG	5.82	126.21	113.40
1	A	176	VAL	CB-CA-C	5.78	122.38	111.40
1	B	118	ARG	CD-NE-CZ	5.77	131.68	123.60
1	A	81	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	220	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	A	262	PHE	CB-CG-CD1	5.69	124.78	120.80
1	B	22	CYS	C-N-CA	-5.68	110.36	122.30
1	A	137	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	5	ASP	N-CA-CB	5.67	120.81	110.60
1	B	18	ALA	N-CA-CB	5.64	117.99	110.10
1	A	169	PHE	CB-CG-CD1	-5.64	116.85	120.80
1	A	239	GLU	N-CA-CB	-5.56	100.59	110.60
1	A	262	PHE	CB-CG-CD2	-5.54	116.92	120.80
1	B	111	ASP	OD1-CG-OD2	-5.53	112.79	123.30
1	B	175	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	94	ASN	O-C-N	-5.49	113.92	122.70
1	B	81	ARG	CG-CD-NE	5.48	123.30	111.80
1	A	21	TYR	CZ-CE2-CD2	-5.46	114.89	119.80
1	A	56	GLU	OE1-CD-OE2	5.41	129.79	123.30
1	A	129	GLU	CG-CD-OE2	-5.40	107.50	118.30
1	B	194	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	B	244	THR	CA-C-N	5.36	126.92	116.20
1	A	205	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
1	B	33	ASN	CA-CB-CG	-5.35	101.63	113.40
1	A	68	ALA	CB-CA-C	-5.31	102.13	110.10
1	B	25	ASN	CB-CG-OD1	-5.29	111.01	121.60
1	A	83	SER	CA-C-O	5.29	131.22	120.10
1	A	125	ARG	CG-CD-NE	5.29	122.90	111.80
1	B	21	TYR	CA-CB-CG	5.29	123.44	113.40
1	A	232	ARG	CA-CB-CG	5.28	125.03	113.40
1	B	211	PHE	N-CA-CB	5.28	120.09	110.60
1	A	46	LYS	CA-CB-CG	5.25	124.94	113.40
1	A	51	PHE	CB-CA-C	-5.24	99.91	110.40
1	B	111	ASP	CB-CA-C	5.22	120.83	110.40
1	B	139	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	167	ASP	CB-CG-OD2	-5.18	113.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	16	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	244	THR	C-N-CA	-5.17	111.44	122.30
1	B	216	SER	O-C-N	5.16	130.95	122.70
1	A	1	GLU	CA-C-N	5.15	128.53	117.20
1	B	232	ARG	CD-NE-CZ	-5.14	116.41	123.60
1	A	134	GLU	CA-CB-CG	5.13	124.68	113.40
1	B	85	SER	N-CA-CB	5.10	118.16	110.50
1	B	167	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	205	ARG	CA-CB-CG	5.09	124.59	113.40
1	B	16	TYR	CZ-CE2-CD2	-5.08	115.22	119.80
1	B	133	ARG	NH1-CZ-NH2	5.07	124.97	119.40
1	B	195	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	B	1	GLU	CB-CA-C	5.03	120.46	110.40
1	A	138	TYR	CB-CG-CD1	5.03	124.02	121.00
1	B	103	ILE	CA-CB-CG2	5.02	120.94	110.90
1	B	209	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	GLU	Mainchain
1	A	154	VAL	Mainchain
1	A	156	GLY	Mainchain
1	A	170	SER	Mainchain
1	A	192	THR	Mainchain
1	A	20	ALA	Mainchain
1	A	203	VAL	Mainchain
1	A	204	PRO	Mainchain
1	A	207	PRO	Mainchain
1	A	216	SER	Mainchain
1	A	22	CYS	Mainchain
1	A	24	LYS	Mainchain
1	A	241	ILE	Mainchain
1	A	245	GLY	Mainchain
1	A	253	PRO	Mainchain
1	A	254	ASP	Mainchain
1	A	26	ASN	Mainchain
1	A	33	ASN	Mainchain
1	A	44	VAL	Mainchain
1	A	47	ALA	Mainchain
1	A	51	PHE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	53	TYR	Mainchain
1	A	66	PHE	Mainchain
1	A	68	ALA	Mainchain
1	A	76	ILE	Mainchain
1	A	93	LEU	Mainchain
1	B	100	ILE	Mainchain
1	B	101	ASN	Mainchain
1	B	124	LEU	Mainchain
1	B	137	ASP	Mainchain
1	B	158	ASP	Mainchain
1	B	169	PHE	Mainchain
1	B	17	SER	Mainchain
1	B	175	ARG	Mainchain
1	B	197	THR	Mainchain
1	B	201	ASP	Mainchain
1	B	203	VAL	Mainchain
1	B	218	PRO	Mainchain
1	B	229	PRO	Mainchain
1	B	234	ASP	Mainchain
1	B	237	LYS	Mainchain
1	B	238	ILE	Mainchain
1	B	239	GLU	Mainchain
1	B	241	ILE	Mainchain
1	B	244	THR	Mainchain
1	B	255	ILE	Mainchain
1	B	268	CYS	Mainchain
1	B	34	ILE	Mainchain
1	B	41	CYS	Mainchain
1	B	94	ASN	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	1964	57	0
1	B	2071	0	1964	53	0
2	A	99	0	0	6	0
2	B	143	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4384	0	3928	109	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 14.

All (109) 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:232:ARG:HD2	2:A:272:HOH:O	1.73	0.89
1:A:1:GLU:HB2	1:A:235:ILE:O	1.81	0.80
1:A:157:ALA:HB2	1:A:185:LEU:HD21	1.68	0.74
1:A:209:ARG:HD3	2:B:330:HOH:O	1.87	0.73
1:A:28:ALA:HA	2:A:326:HOH:O	1.92	0.69
1:A:84:ARG:HB2	1:A:84:ARG:HH11	1.62	0.65
1:A:245:GLY:HA2	1:A:249:GLN:NE2	2.11	0.65
1:A:25:ASN:HB3	1:A:51:PHE:CZ	2.33	0.64
1:A:4:GLN:HE21	1:A:232:ARG:HG2	1.63	0.63
1:A:204:PRO:HB2	1:A:247:ASN:OD1	2.00	0.62
1:A:232:ARG:HG3	2:A:279:HOH:O	1.98	0.62
1:A:53:TYR:CD2	1:A:127:LYS:HD3	2.35	0.62
1:A:25:ASN:HB3	1:A:51:PHE:HZ	1.65	0.61
1:B:95:PHE:CD1	1:B:207:PRO:HB3	2.37	0.60
1:B:1:GLU:CD	1:B:233:ASN:HA	2.22	0.60
1:A:195:ARG:NH1	1:A:219:GLU:HB2	2.17	0.59
1:B:156:GLY:O	1:B:160:ARG:HD2	2.01	0.59
1:B:125:ARG:HB2	1:B:159:LEU:HD13	1.84	0.59
1:B:134:GLU:HG3	2:B:395:HOH:O	2.03	0.58
1:B:81:ARG:HD2	1:B:82:GLY:O	2.04	0.58
1:B:23:GLY:HA3	1:B:36:CYS:HA	1.86	0.57
1:B:98:LYS:HB3	1:B:111:ASP:HB2	1.87	0.56
1:B:87:GLU:OE1	1:B:88:ASN:N	2.27	0.55
1:A:175:ARG:NH2	1:A:207:PRO:O	2.37	0.55
1:A:28:ALA:HB1	1:A:29:PRO:HD2	1.88	0.54
1:B:254:ASP:OD1	1:B:256:PRO:HD2	2.08	0.54
1:B:198:HIS:NE2	1:B:224:SER:O	2.33	0.54
1:B:25:ASN:HA	1:B:51:PHE:CZ	2.44	0.53
1:A:20:ALA:O	1:A:81:ARG:HG3	2.09	0.53
1:A:245:GLY:H	1:A:249:GLN:HG3	1.74	0.53
1:A:160:ARG:NH1	1:A:188:GLN:OE1	2.40	0.52
1:A:125:ARG:HG2	1:A:125:ARG:HH11	1.75	0.52
1:A:34:ILE:HG12	1:A:51:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:THR:HA	1:A:169:PHE:O	2.11	0.51
1:B:108:ARG:HG3	1:B:178:ASN:ND2	2.26	0.51
1:B:134:GLU:HB3	1:B:135:HIS:CD2	2.46	0.50
1:A:64:THR:HG21	1:A:81:ARG:NH2	2.27	0.50
1:A:220:TYR:OH	1:A:237:LYS:HE3	2.11	0.50
1:A:1:GLU:HG3	1:A:236:VAL:CG2	2.42	0.50
1:A:205:ARG:NH1	1:A:247:ASN:O	2.45	0.49
1:B:52:LEU:HD11	1:B:69:LEU:HB2	1.94	0.49
1:A:108:ARG:HG3	1:A:178:ASN:ND2	2.28	0.49
1:B:143:THR:HA	1:B:169:PHE:O	2.13	0.49
1:B:1:GLU:HB3	1:B:235:ILE:O	2.12	0.48
1:A:33:ASN:HD22	1:A:50:THR:HG22	1.79	0.48
1:A:97:LEU:HD12	1:A:97:LEU:N	2.28	0.48
1:B:56:GLU:O	1:B:57:ASP:HB2	2.14	0.48
1:A:108:ARG:HG3	1:A:178:ASN:HD21	1.78	0.48
1:A:253:PRO:HD3	1:B:211:PHE:HA	1.96	0.47
1:A:81:ARG:HD2	1:A:82:GLY:O	2.14	0.47
1:B:221:TRP:CE3	1:B:246:GLY:HA2	2.49	0.47
1:B:196:ILE:HA	1:B:220:TYR:O	2.14	0.47
1:A:29:PRO:HD3	2:A:326:HOH:O	2.14	0.47
1:A:245:GLY:HA2	1:A:249:GLN:CD	2.34	0.47
1:B:26:ASN:ND2	1:B:26:ASN:H	2.12	0.47
1:B:25:ASN:OD1	1:B:66:PHE:CD2	2.68	0.47
1:B:28:ALA:HB1	1:B:29:PRO:HD2	1.96	0.46
1:A:202:ILE:O	1:A:205:ARG:HB2	2.16	0.46
1:B:20:ALA:O	1:B:81:ARG:HG3	2.16	0.46
1:A:179:ARG:O	1:A:182:ALA:HB3	2.16	0.46
1:A:1:GLU:HG3	1:A:236:VAL:HG22	1.97	0.46
1:A:49:ALA:HA	1:A:69:LEU:O	2.16	0.45
1:A:13:PHE:CE1	1:A:141:VAL:HG11	2.51	0.45
1:A:245:GLY:HA2	1:A:249:GLN:CG	2.47	0.45
1:B:24:LYS:HB3	2:B:365:HOH:O	2.17	0.45
1:A:202:ILE:HB	1:A:253:PRO:HB2	1.99	0.45
1:A:193:LEU:HD12	1:A:194:TYR:N	2.32	0.44
1:B:85:SER:HB3	1:B:87:GLU:OE1	2.17	0.44
1:B:85:SER:HB3	1:B:87:GLU:OE2	2.16	0.44
1:B:157:ALA:HB2	1:B:185:LEU:HD21	1.99	0.44
1:B:232:ARG:HH11	1:B:232:ARG:HD3	1.47	0.44
1:B:221:TRP:CD2	1:B:246:GLY:HA2	2.52	0.44
1:B:176:VAL:HG12	1:B:181:PHE:HE2	1.82	0.43
1:A:35:THR:HG21	2:A:339:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:HIS:O	1:A:199:THR:C	2.56	0.43
1:B:97:LEU:HB2	2:B:408:HOH:O	2.18	0.43
1:B:133:ARG:HH11	1:B:133:ARG:HD3	1.68	0.43
1:B:198:HIS:N	1:B:261:TYR:OH	2.51	0.43
1:A:125:ARG:NH1	1:A:129:GLU:OE2	2.52	0.43
1:A:146:SER:O	1:A:149:GLY:N	2.49	0.43
1:B:25:ASN:HA	1:B:51:PHE:HZ	1.82	0.43
1:B:1:GLU:OE1	1:B:1:GLU:N	2.43	0.43
1:A:73:ASN:O	1:A:74:LYS:HB2	2.18	0.43
1:B:179:ARG:O	1:B:183:GLU:HB2	2.19	0.43
1:B:255:ILE:HB	1:B:256:PRO:HD3	2.01	0.42
1:B:176:VAL:HG12	1:B:181:PHE:CE2	2.55	0.42
1:B:94:ASN:O	1:B:96:ASP:N	2.52	0.42
1:A:84:ARG:HH11	1:A:84:ARG:CB	2.28	0.42
1:A:149:GLY:HA3	1:A:173:ALA:HB2	2.01	0.42
1:A:110:HIS:O	1:A:114:THR:HB	2.20	0.42
1:B:26:ASN:O	1:B:27:ASP:OD1	2.38	0.42
1:A:218:PRO:HG3	1:A:237:LYS:HE2	2.02	0.41
1:B:49:ALA:HA	1:B:69:LEU:O	2.20	0.41
1:B:198:HIS:O	1:B:199:THR:C	2.58	0.41
1:B:206:LEU:HA	1:B:207:PRO:C	2.39	0.41
1:A:1:GLU:HB3	2:A:303:HOH:O	2.19	0.41
1:B:128:VAL:O	1:B:132:VAL:HG23	2.19	0.41
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.90	0.41
1:A:4:GLN:NE2	1:A:232:ARG:HG2	2.32	0.41
1:A:55:PHE:HE1	1:A:63:VAL:HG12	1.86	0.41
1:B:123:THR:O	1:B:126:GLN:HB3	2.21	0.41
1:B:133:ARG:O	1:B:136:PRO:HD3	2.20	0.41
1:A:64:THR:HG21	1:A:81:ARG:CZ	2.52	0.40
1:A:88:ASN:O	1:A:92:ASN:ND2	2.50	0.40
1:B:23:GLY:O	1:B:25:ASN:N	2.54	0.40
1:B:201:ASP:OD1	1:B:258:HIS:HB2	2.21	0.40
1:B:21:TYR:CE2	1:B:266:GLY:HA2	2.57	0.40
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.87	0.40
1:B:78:LEU:HB3	1:B:142:PHE:CD1	2.56	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 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%)	253 (95%)	12 (4%)	2 (1%)	22 43
1	B	267/269 (99%)	246 (92%)	17 (6%)	4 (2%)	10 21
All	All	534/538 (99%)	499 (93%)	29 (5%)	6 (1%)	14 30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	ALA
1	A	62	ASP
1	A	199	THR
1	B	199	THR
1	B	95	PHE
1	B	23	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 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%)	194 (88%)	26 (12%)	5 9
1	B	220/220 (100%)	199 (90%)	21 (10%)	8 16
All	All	440/440 (100%)	393 (89%)	47 (11%)	6 12

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	25	ASN
1	A	27	ASP
1	A	46	LYS
1	A	60	VAL
1	A	83	SER
1	A	84	ARG
1	A	87	GLU
1	A	94	ASN
1	A	97	LEU
1	A	98	LYS
1	A	100	ILE
1	A	101	ASN
1	A	102	ASP
1	A	105	SER
1	A	115	SER
1	A	118	ARG
1	A	162	ASN
1	A	176	VAL
1	A	193	LEU
1	A	209	ARG
1	A	214	SER
1	A	216	SER
1	A	224	SER
1	A	232	ARG
1	A	241	ILE
1	B	26	ASN
1	B	27	ASP
1	B	87	GLU
1	B	99	GLU
1	B	102	ASP
1	B	104	CYS
1	B	105	SER
1	B	111	ASP
1	B	118	ARG
1	B	125	ARG
1	B	127	LYS
1	B	134	GLU
1	B	137	ASP
1	B	146	SER
1	B	179	ARG
1	B	183	GLU
1	B	205	ARG

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Mol	Chain	Res	Type
1	B	210	GLU
1	B	214	SER
1	B	232	ARG
1	B	252	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	33	ASN
1	A	88	ASN
1	A	94	ASN
1	A	162	ASN
1	A	249	GLN
1	B	25	ASN
1	B	26	ASN
1	B	135	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 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)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.