Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:07 PM EDT

PDB ID	:	1DU4
Title	:	THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE OTHER STRUCTURE DETAILS
Authors	:	Brozozowski, A.M.; Savage, H.
Deposited on	:	2000-01-14
Resolution	:	2.50 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:

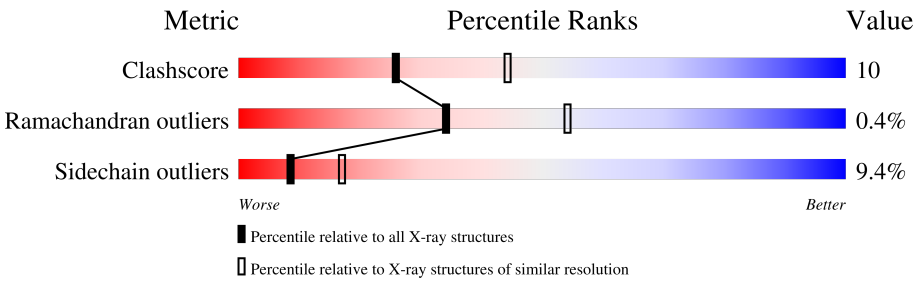
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	71% 20% 6% •
1	B	269	71% 22% 5% •
1	C	269	72% 21% 6%
1	D	269	71% 24% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8935 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
1	C	269	2071	1303	359	403	6	0	0	0
1	D	269	2071	1303	359	403	6	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	179	179	179	0	0
2	B	162	162	162	0	0
2	C	173	173	173	0	0
2	D	137	137	137	0	0

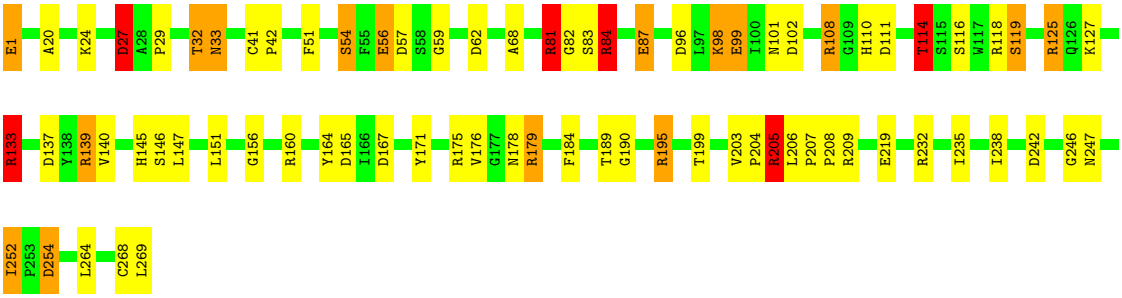
3 Residue-property plots (i)

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.

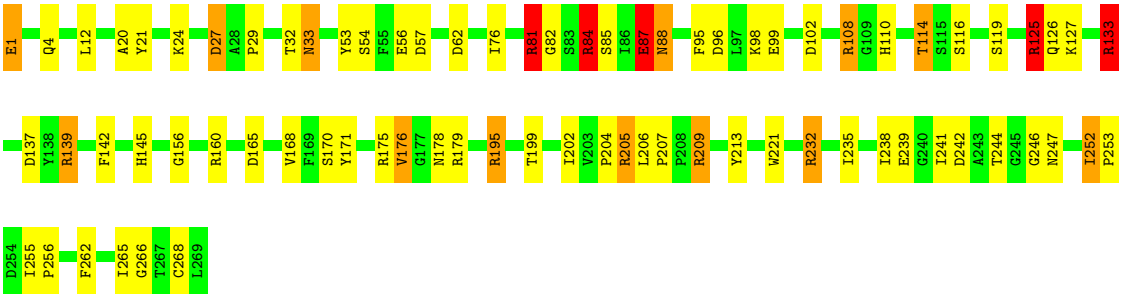
• Molecule 1: LIPASE

Chain A:



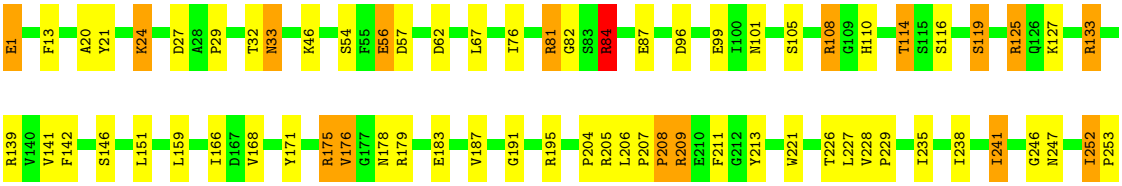
• Molecule 1: LIPASE

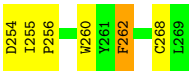
Chain B:



• Molecule 1: LIPASE

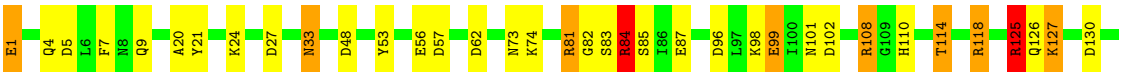
Chain C:

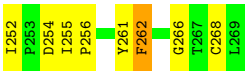




• Molecule 1: LIPASE

Chain D:





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	85.56Å 171.16Å 77.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.2 (30.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8935	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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	0.60	0/2121	1.87	44/2887 (1.5%)
1	B	0.56	0/2121	1.85	37/2887 (1.3%)
1	C	0.56	0/2121	1.63	23/2887 (0.8%)
1	D	0.54	0/2121	1.73	32/2887 (1.1%)
All	All	0.57	0/8484	1.77	136/11548 (1.2%)

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	2
1	B	0	2
1	C	0	1
All	All	0	5

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	ARG	CD-NE-CZ	29.21	164.49	123.60
1	D	175	ARG	CD-NE-CZ	28.89	164.04	123.60
1	C	175	ARG	CD-NE-CZ	27.16	161.62	123.60
1	C	195	ARG	CD-NE-CZ	25.39	159.14	123.60
1	B	84	ARG	NE-CZ-NH2	-24.81	107.89	120.30
1	A	84	ARG	NE-CZ-NH1	23.31	131.96	120.30
1	A	195	ARG	NE-CZ-NH2	-23.06	108.77	120.30
1	D	175	ARG	NE-CZ-NH2	-22.55	109.03	120.30
1	B	205	ARG	NE-CZ-NH1	22.53	131.57	120.30
1	B	175	ARG	NE-CZ-NH1	-21.48	109.56	120.30
1	C	195	ARG	NE-CZ-NH2	-20.93	109.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	87	GLU	OE1-CD-OE2	20.66	148.09	123.30
1	D	81	ARG	NE-CZ-NH1	20.66	130.63	120.30
1	A	84	ARG	NE-CZ-NH2	-19.58	110.51	120.30
1	C	205	ARG	NE-CZ-NH1	18.71	129.65	120.30
1	B	195	ARG	CD-NE-CZ	17.62	148.27	123.60
1	A	205	ARG	CD-NE-CZ	17.62	148.26	123.60
1	D	195	ARG	CD-NE-CZ	17.42	147.99	123.60
1	B	205	ARG	NE-CZ-NH2	-16.80	111.90	120.30
1	B	84	ARG	NE-CZ-NH1	16.27	128.43	120.30
1	B	195	ARG	NE-CZ-NH2	-16.26	112.17	120.30
1	B	81	ARG	NE-CZ-NH1	16.04	128.32	120.30
1	A	175	ARG	NE-CZ-NH2	-15.41	112.59	120.30
1	A	195	ARG	CD-NE-CZ	15.36	145.10	123.60
1	D	84	ARG	NE-CZ-NH1	14.74	127.67	120.30
1	D	205	ARG	CD-NE-CZ	14.41	143.77	123.60
1	B	179	ARG	NE-CZ-NH2	-14.11	113.25	120.30
1	B	209	ARG	NE-CZ-NH2	-13.20	113.70	120.30
1	B	27	ASP	CB-CG-OD2	-12.44	107.11	118.30
1	B	205	ARG	CD-NE-CZ	12.44	141.01	123.60
1	A	81	ARG	NE-CZ-NH1	12.28	126.44	120.30
1	A	205	ARG	NE-CZ-NH1	12.11	126.35	120.30
1	D	179	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	D	179	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	A	27	ASP	CB-CG-OD2	11.22	128.40	118.30
1	D	205	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	D	84	ARG	NE-CZ-NH2	-11.03	114.78	120.30
1	A	108	ARG	NE-CZ-NH2	-10.91	114.84	120.30
1	D	108	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	C	81	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	C	205	ARG	CD-NE-CZ	9.66	137.12	123.60
1	D	81	ARG	NE-CZ-NH2	-9.41	115.60	120.30
1	A	133	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	195	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	D	209	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	B	232	ARG	NE-CZ-NH1	-8.97	115.81	120.30
1	A	179	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	D	108	ARG	CD-NE-CZ	8.59	135.63	123.60
1	B	87	GLU	CG-CD-OE2	-8.46	101.38	118.30
1	D	175	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	205	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	B	232	ARG	CD-NE-CZ	8.35	135.28	123.60
1	A	96	ASP	CB-CG-OD1	8.30	125.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	84	ARG	CD-NE-CZ	8.27	135.17	123.60
1	D	171	TYR	CB-CG-CD2	8.25	125.95	121.00
1	A	139	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	D	195	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	C	195	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	81	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	209	ARG	CD-NE-CZ	7.67	134.34	123.60
1	D	160	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	219	GLU	OE1-CD-OE2	-7.57	114.22	123.30
1	C	179	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	137	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	B	175	ARG	CD-NE-CZ	7.49	134.09	123.60
1	A	242	ASP	CB-CG-OD2	7.48	125.03	118.30
1	C	175	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	B	175	ARG	NH1-CZ-NH2	7.42	127.56	119.40
1	B	87	GLU	CB-CG-CD	-7.39	94.25	114.20
1	A	209	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	137	ASP	CB-CG-OD1	7.27	124.84	118.30
1	D	7	PHE	CB-CG-CD1	-7.26	115.72	120.80
1	D	205	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	125	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	139	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	C	133	ARG	CD-NE-CZ	6.70	132.98	123.60
1	A	133	ARG	CD-NE-CZ	6.68	132.95	123.60
1	D	171	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	A	242	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	A	125	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	133	ARG	NH1-CZ-NH2	-6.49	112.26	119.40
1	A	254	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	96	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	21	TYR	CB-CG-CD2	6.46	124.88	121.00
1	A	84	ARG	CD-NE-CZ	6.45	132.63	123.60
1	A	179	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	81	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	D	175	ARG	NH1-CZ-NH2	6.40	126.44	119.40
1	D	160	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	232	ARG	CD-NE-CZ	6.37	132.52	123.60
1	B	125	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	C	171	TYR	CB-CG-CD1	-6.27	117.24	121.00
1	C	108	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	A	195	ARG	NH1-CZ-NH2	6.22	126.24	119.40
1	A	96	ASP	CB-CG-OD2	-6.20	112.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	84	ARG	CD-NE-CZ	6.19	132.27	123.60
1	D	219	GLU	OE1-CD-OE2	-6.16	115.91	123.30
1	D	201	ASP	CB-CG-OD2	6.07	123.77	118.30
1	B	176	VAL	CG1-CB-CG2	6.07	120.61	110.90
1	B	27	ASP	OD1-CG-OD2	6.04	134.77	123.30
1	A	171	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	B	137	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	171	TYR	CB-CG-CD2	5.89	124.54	121.00
1	C	96	ASP	CB-CG-OD1	5.89	123.60	118.30
1	C	195	ARG	NH1-CZ-NH2	5.88	125.87	119.40
1	C	205	ARG	NH1-CZ-NH2	-5.86	112.96	119.40
1	B	171	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	167	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	205	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	21	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	D	118	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	B	195	ARG	NH1-CZ-NH2	5.66	125.63	119.40
1	B	179	ARG	NH1-CZ-NH2	5.66	125.63	119.40
1	D	96	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	84	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	125	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	175	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	118	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	48	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	133	ARG	CD-NE-CZ	5.36	131.10	123.60
1	B	108	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	264	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	C	108	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	C	262	PHE	C-N-CA	5.27	133.37	122.30
1	A	167	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	C	209	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	114	THR	N-CA-CB	-5.18	100.45	110.30
1	B	262	PHE	C-N-CA	5.18	133.18	122.30
1	B	175	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	165	ASP	CB-CG-OD1	5.15	122.93	118.30
1	D	81	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	C	176	VAL	N-CA-CB	-5.11	100.25	111.50
1	A	209	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	244	THR	CA-C-N	5.10	126.39	116.20
1	A	184	PHE	CB-CG-CD1	-5.04	117.27	120.80
1	B	133	ARG	CD-NE-CZ	5.01	130.62	123.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	VAL	Mainchain
1	A	68	ALA	Mainchain
1	B	170	SER	Mainchain
1	B	76	ILE	Mainchain
1	C	208	PRO	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	44	0
1	B	2071	0	1965	39	0
1	C	2071	0	1965	44	0
1	D	2071	0	1965	42	0
2	A	179	0	0	6	0
2	B	162	0	0	8	0
2	C	173	0	0	5	0
2	D	137	0	0	6	0
All	All	8935	0	7860	169	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 (169) 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:33:ASN:HD22	1:A:33:ASN:H	1.22	0.86
1:B:20:ALA:HB1	1:B:81:ARG:HB2	1.64	0.80
1:B:87:GLU:HG2	2:B:430:HOH:O	1.83	0.77
1:C:20:ALA:HB1	1:C:81:ARG:HB2	1.69	0.74
1:C:84:ARG:HD3	1:C:84:ARG:O	1.86	0.74
1:B:81:ARG:HD3	1:B:82:GLY:O	1.87	0.73
1:C:209:ARG:HD2	1:C:213:TYR:O	1.90	0.71
1:B:84:ARG:O	1:B:84:ARG:HD3	1.90	0.71
1:A:84:ARG:O	1:A:84:ARG:HD3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:HIS:O	1:A:114:THR:HB	1.90	0.70
1:C:27:ASP:HB2	2:C:330:HOH:O	1.89	0.70
1:A:81:ARG:HD3	1:A:82:GLY:O	1.92	0.70
1:A:99:GLU:OE1	1:A:101:ASN:ND2	2.24	0.69
1:A:33:ASN:HD22	1:A:33:ASN:N	1.92	0.68
1:C:125:ARG:HD3	1:C:159:LEU:HD22	1.76	0.67
1:D:1:GLU:HB2	1:D:235:ILE:O	1.95	0.66
1:C:110:HIS:O	1:C:114:THR:HB	1.95	0.65
1:D:208:PRO:HD2	1:D:211:PHE:HD1	1.60	0.65
1:A:20:ALA:HB1	1:A:81:ARG:HB2	1.77	0.65
1:A:108:ARG:HG3	1:A:178:ASN:ND2	2.12	0.65
1:C:33:ASN:HD22	1:C:33:ASN:H	1.45	0.63
1:C:81:ARG:HD3	1:C:82:GLY:O	1.98	0.63
1:B:232:ARG:HD3	2:B:281:HOH:O	1.99	0.61
1:D:125:ARG:HD3	1:D:159:LEU:HD22	1.83	0.60
1:D:84:ARG:NH2	1:D:268:CYS:O	2.34	0.60
1:D:33:ASN:H	1:D:33:ASN:HD22	1.49	0.59
1:C:108:ARG:HG3	1:C:178:ASN:ND2	2.18	0.58
1:A:206:LEU:HA	1:A:207:PRO:C	2.25	0.58
1:C:183:GLU:HG3	1:C:241:ILE:HD12	1.85	0.57
1:C:133:ARG:HG2	1:C:133:ARG:HH11	1.70	0.57
1:B:239:GLU:HG3	2:B:296:HOH:O	2.05	0.57
1:D:110:HIS:O	1:D:114:THR:HB	2.04	0.57
1:C:238:ILE:HD13	1:C:246:GLY:CA	2.35	0.56
1:B:85:SER:OG	1:B:88:ASN:HB2	2.04	0.56
1:D:84:ARG:O	1:D:84:ARG:HD3	2.06	0.56
1:B:110:HIS:O	1:B:114:THR:HB	2.05	0.56
1:A:29:PRO:O	1:A:32:THR:HB	2.06	0.55
1:C:84:ARG:NH2	1:C:268:CYS:O	2.39	0.55
1:A:1:GLU:HB2	1:A:235:ILE:O	2.05	0.55
1:A:81:ARG:NH2	1:A:84:ARG:HG2	2.21	0.55
1:C:1:GLU:HB2	1:C:235:ILE:O	2.07	0.55
1:C:133:ARG:HD3	2:C:376:HOH:O	2.06	0.55
1:B:126:GLN:HB2	2:B:412:HOH:O	2.06	0.55
1:A:165:ASP:OD1	1:A:190:GLY:HA2	2.07	0.55
1:B:133:ARG:HG2	1:B:133:ARG:HH11	1.72	0.55
1:D:108:ARG:HG3	1:D:178:ASN:ND2	2.22	0.54
1:A:133:ARG:HH11	1:A:133:ARG:HG3	1.72	0.54
1:C:116:SER:O	1:C:119:SER:HB2	2.08	0.54
1:A:87:GLU:HB3	2:A:321:HOH:O	2.07	0.54
1:D:85:SER:HB2	2:D:293:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:OD1	1:A:62:ASP:HB3	2.08	0.54
1:D:73:ASN:O	1:D:74:LYS:HB2	2.09	0.52
1:B:1:GLU:HB2	1:B:235:ILE:O	2.09	0.52
1:A:57:ASP:HA	1:A:62:ASP:HA	1.91	0.52
1:C:206:LEU:HA	1:C:207:PRO:C	2.31	0.51
1:C:13:PHE:CE1	1:C:141:VAL:HG11	2.46	0.51
1:D:20:ALA:HB1	1:D:81:ARG:HB2	1.93	0.51
1:D:53:TYR:CD1	1:D:127:LYS:HE3	2.46	0.51
1:D:189:THR:HA	2:D:351:HOH:O	2.10	0.50
1:B:84:ARG:NH2	1:B:268:CYS:O	2.40	0.50
1:C:252:ILE:HD12	1:C:253:PRO:O	2.12	0.50
1:D:5:ASP:O	1:D:9:GLN:HG3	2.11	0.50
1:A:33:ASN:H	1:A:33:ASN:ND2	2.02	0.50
1:D:204:PRO:HB2	1:D:247:ASN:OD1	2.12	0.50
1:A:133:ARG:HH11	1:A:133:ARG:CG	2.25	0.50
1:B:29:PRO:O	1:B:32:THR:HB	2.12	0.50
1:B:252:ILE:HD11	2:B:340:HOH:O	2.11	0.49
1:B:125:ARG:HG2	2:B:371:HOH:O	2.11	0.49
1:D:261:TYR:O	1:D:262:PHE:HB2	2.12	0.49
1:A:156:GLY:O	1:A:160:ARG:HG3	2.12	0.49
1:C:101:ASN:OD1	1:C:105:SER:HA	2.12	0.49
1:D:179:ARG:HD2	1:D:241:ILE:HG21	1.95	0.49
1:A:204:PRO:HB2	1:A:247:ASN:OD1	2.13	0.48
1:D:130:ASP:O	1:D:133:ARG:HG2	2.14	0.48
1:C:238:ILE:HD13	1:C:246:GLY:HA3	1.95	0.48
1:B:12:LEU:HD13	2:B:310:HOH:O	2.14	0.48
1:C:228:VAL:CG1	1:C:229:PRO:HD2	2.43	0.48
1:D:27:ASP:HB2	2:D:288:HOH:O	2.13	0.48
1:B:238:ILE:HD13	1:B:246:GLY:HA3	1.96	0.48
1:D:246:GLY:O	1:D:249:GLN:HG3	2.14	0.48
1:B:206:LEU:HA	1:B:207:PRO:C	2.34	0.47
1:A:84:ARG:NH2	1:A:268:CYS:O	2.42	0.47
1:A:41:CYS:N	1:A:42:PRO:CD	2.78	0.47
1:A:32:THR:HG22	1:A:51:PHE:CD2	2.50	0.47
1:C:204:PRO:HB2	1:C:247:ASN:OD1	2.14	0.47
1:A:98:LYS:HG2	1:A:111:ASP:HA	1.97	0.47
1:A:238:ILE:HD13	1:A:246:GLY:CA	2.45	0.47
1:D:4:GLN:OE1	1:D:232:ARG:HD2	2.15	0.46
1:B:57:ASP:HA	1:B:62:ASP:HA	1.98	0.46
1:B:145:HIS:HB2	1:B:265:ILE:HD11	1.97	0.46
1:D:33:ASN:ND2	1:D:33:ASN:N	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:SER:O	1:A:119:SER:HB2	2.15	0.46
1:A:145:HIS:CE1	1:A:146:SER:HB2	2.50	0.46
1:B:252:ILE:HD12	1:B:253:PRO:O	2.15	0.46
1:D:20:ALA:O	1:D:81:ARG:HG3	2.16	0.46
1:D:81:ARG:HD2	1:D:82:GLY:O	2.16	0.46
1:A:252:ILE:HD11	2:A:317:HOH:O	2.16	0.46
1:C:57:ASP:HA	1:C:62:ASP:HA	1.97	0.46
1:C:29:PRO:O	1:C:32:THR:HB	2.15	0.46
1:D:206:LEU:HA	1:D:207:PRO:C	2.36	0.46
1:A:54:SER:HB2	2:A:396:HOH:O	2.15	0.45
1:D:21:TYR:CD2	1:D:266:GLY:HA2	2.52	0.45
1:B:207:PRO:HG2	1:B:213:TYR:CZ	2.52	0.45
1:B:116:SER:O	1:B:119:SER:HB2	2.16	0.45
1:B:255:ILE:N	1:B:256:PRO:CD	2.79	0.45
1:D:207:PRO:HG2	1:D:213:TYR:CZ	2.51	0.45
1:A:205:ARG:HG3	2:A:295:HOH:O	2.17	0.45
1:C:226:THR:HG22	1:C:227:LEU:HG	1.99	0.45
1:A:87:GLU:H	1:A:87:GLU:CD	2.20	0.45
1:B:57:ASP:OD1	1:B:62:ASP:HB3	2.17	0.45
1:B:108:ARG:HG3	1:B:178:ASN:ND2	2.31	0.45
1:D:179:ARG:HB3	2:D:337:HOH:O	2.15	0.45
1:B:33:ASN:HD22	1:B:33:ASN:H	1.65	0.45
1:D:160:ARG:NH1	1:D:188:GLN:OE1	2.50	0.45
1:A:206:LEU:HD23	1:A:208:PRO:HD3	1.98	0.44
1:B:21:TYR:CE2	1:B:266:GLY:HA2	2.53	0.44
1:D:126:GLN:HG2	2:D:381:HOH:O	2.17	0.44
1:C:175:ARG:HD2	1:C:213:TYR:HB3	2.00	0.44
1:A:32:THR:HG22	1:A:51:PHE:HD2	1.81	0.44
1:B:53:TYR:CD2	1:B:127:LYS:HD3	2.52	0.44
1:B:142:PHE:O	1:B:168:VAL:HA	2.17	0.44
1:A:27:ASP:OD1	1:A:56:GLU:OE1	2.35	0.44
1:C:46:LYS:HE2	2:C:379:HOH:O	2.18	0.44
1:C:33:ASN:H	1:C:33:ASN:ND2	2.13	0.44
1:B:4:GLN:OE1	1:B:232:ARG:HD2	2.18	0.44
1:D:99:GLU:OE1	1:D:101:ASN:ND2	2.50	0.43
1:D:99:GLU:HB2	2:D:353:HOH:O	2.17	0.43
1:D:57:ASP:HA	1:D:62:ASP:HA	2.01	0.43
1:D:175:ARG:HG2	1:D:215:HIS:CE1	2.52	0.43
1:C:67:LEU:HD11	1:C:76:ILE:HG22	2.01	0.43
1:D:87:GLU:H	1:D:87:GLU:CD	2.22	0.43
1:D:133:ARG:HG2	1:D:133:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HD12	1:A:147:LEU:O	2.18	0.43
1:B:156:GLY:O	1:B:160:ARG:HG3	2.18	0.43
1:D:166:ILE:O	1:D:191:GLY:HA3	2.19	0.43
1:C:33:ASN:ND2	1:C:33:ASN:N	2.66	0.43
1:D:81:ARG:CD	1:D:82:GLY:O	2.66	0.43
1:A:1:GLU:HG3	1:A:235:ILE:O	2.19	0.42
1:B:241:ILE:O	1:B:242:ASP:HB2	2.18	0.42
1:B:202:ILE:HB	1:B:253:PRO:HB2	2.00	0.42
1:C:24:LYS:HG2	2:C:419:HOH:O	2.18	0.42
1:D:33:ASN:H	1:D:33:ASN:ND2	2.15	0.42
1:D:221:TRP:CE3	1:D:246:GLY:HA2	2.54	0.42
1:A:81:ARG:CD	1:A:82:GLY:O	2.63	0.42
1:D:255:ILE:N	1:D:256:PRO:CD	2.83	0.42
1:C:166:ILE:O	1:C:191:GLY:HA3	2.20	0.42
1:B:221:TRP:CE3	1:B:246:GLY:HA2	2.55	0.41
1:C:227:LEU:HD23	1:C:260:TRP:CE3	2.55	0.41
1:C:187:VAL:HG22	1:C:187:VAL:O	2.20	0.41
1:A:238:ILE:HD13	1:A:246:GLY:HA3	2.02	0.41
1:A:140:VAL:HG21	1:A:164:TYR:CD2	2.54	0.41
1:C:207:PRO:HB2	1:C:213:TYR:CD1	2.55	0.41
1:A:179:ARG:NH1	2:A:325:HOH:O	2.54	0.41
1:B:195:ARG:HG3	2:B:379:HOH:O	2.21	0.41
1:D:142:PHE:O	1:D:168:VAL:HA	2.21	0.41
1:A:59:GLY:HA3	1:A:119:SER:HB3	2.03	0.41
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.90	0.41
1:A:195:ARG:HG3	2:A:366:HOH:O	2.19	0.41
1:C:27:ASP:OD2	1:C:56:GLU:OE1	2.38	0.41
1:C:253:PRO:HD2	2:C:420:HOH:O	2.20	0.41
1:C:142:PHE:O	1:C:168:VAL:HA	2.21	0.41
1:C:221:TRP:CE3	1:C:246:GLY:HA2	2.56	0.41
1:C:227:LEU:HA	1:C:260:TRP:CE2	2.56	0.41
1:B:202:ILE:O	1:B:205:ARG:HB2	2.20	0.40
1:B:204:PRO:HB2	1:B:247:ASN:OD1	2.20	0.40
1:C:255:ILE:N	1:C:256:PRO:CD	2.85	0.40
1:B:95:PHE:CD1	1:B:207:PRO:HB3	2.57	0.40
1:C:151:LEU:HD23	1:C:151:LEU:HA	1.92	0.40
1:C:208:PRO:HG2	1:C:211:PHE:CE1	2.57	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%)	258 (97%)	8 (3%)	1 (0%)	34	54
1	B	267/269 (99%)	260 (97%)	6 (2%)	1 (0%)	34	54
1	C	267/269 (99%)	257 (96%)	9 (3%)	1 (0%)	34	54
1	D	267/269 (99%)	260 (97%)	6 (2%)	1 (0%)	34	54
All	All	1068/1076 (99%)	1035 (97%)	29 (3%)	4 (0%)	34	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	199	THR
1	A	199	THR
1	D	262	PHE
1	C	262	PHE

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	10
1	B	220/220 (100%)	200 (91%)	20 (9%)	9	18
1	C	220/220 (100%)	202 (92%)	18 (8%)	11	22
1	D	220/220 (100%)	201 (91%)	19 (9%)	10	20
All	All	880/880 (100%)	797 (91%)	83 (9%)	8	17

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	24	LYS
1	A	27	ASP
1	A	32	THR
1	A	33	ASN
1	A	54	SER
1	A	56	GLU
1	A	81	ARG
1	A	83	SER
1	A	84	ARG
1	A	87	GLU
1	A	98	LYS
1	A	99	GLU
1	A	102	ASP
1	A	114	THR
1	A	119	SER
1	A	125	ARG
1	A	127	LYS
1	A	133	ARG
1	A	139	ARG
1	A	176	VAL
1	A	189	THR
1	A	205	ARG
1	A	252	ILE
1	A	254	ASP
1	A	269	LEU
1	B	1	GLU
1	B	24	LYS
1	B	27	ASP
1	B	33	ASN
1	B	54	SER
1	B	56	GLU
1	B	81	ARG
1	B	84	ARG
1	B	87	GLU
1	B	88	ASN
1	B	98	LYS
1	B	99	GLU
1	B	102	ASP
1	B	114	THR
1	B	125	ARG
1	B	133	ARG

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Mol	Chain	Res	Type
1	B	139	ARG
1	B	176	VAL
1	B	209	ARG
1	B	252	ILE
1	C	1	GLU
1	C	24	LYS
1	C	33	ASN
1	C	54	SER
1	C	56	GLU
1	C	84	ARG
1	C	87	GLU
1	C	99	GLU
1	C	114	THR
1	C	119	SER
1	C	125	ARG
1	C	127	LYS
1	C	139	ARG
1	C	146	SER
1	C	176	VAL
1	C	241	ILE
1	C	252	ILE
1	C	254	ASP
1	D	1	GLU
1	D	24	LYS
1	D	33	ASN
1	D	56	GLU
1	D	83	SER
1	D	84	ARG
1	D	98	LYS
1	D	99	GLU
1	D	102	ASP
1	D	114	THR
1	D	118	ARG
1	D	125	ARG
1	D	127	LYS
1	D	139	ARG
1	D	146	SER
1	D	176	VAL
1	D	179	ARG
1	D	252	ILE
1	D	254	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	162	ASN
1	B	33	ASN
1	B	162	ASN
1	C	33	ASN
1	C	135	HIS
1	D	33	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)

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.