



Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 07:26 PM GMT

PDB ID : 2C7B
Title : THE CRYSTAL STRUCTURE OF ESTE1, A NEW THERMOPHILIC AND
THERMOSTABLE CARBOXYLESTERASE CLONED FROM A METAGE-
NOMIC LIBRARY
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Deposited on : 2005-11-21
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

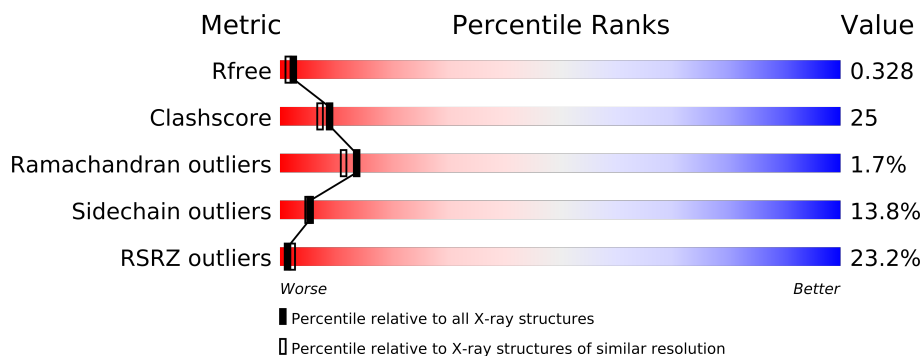
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
R_{free}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	311	
1	B	311	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4607 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CARBOXYLESTERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	Se	12	0	1
			2248	1436	388	419	1	4			
1	B	291	Total	C	N	O	S	Se	0	0	1
			2221	1418	384	414	1	4			

- Molecule 2 is water.

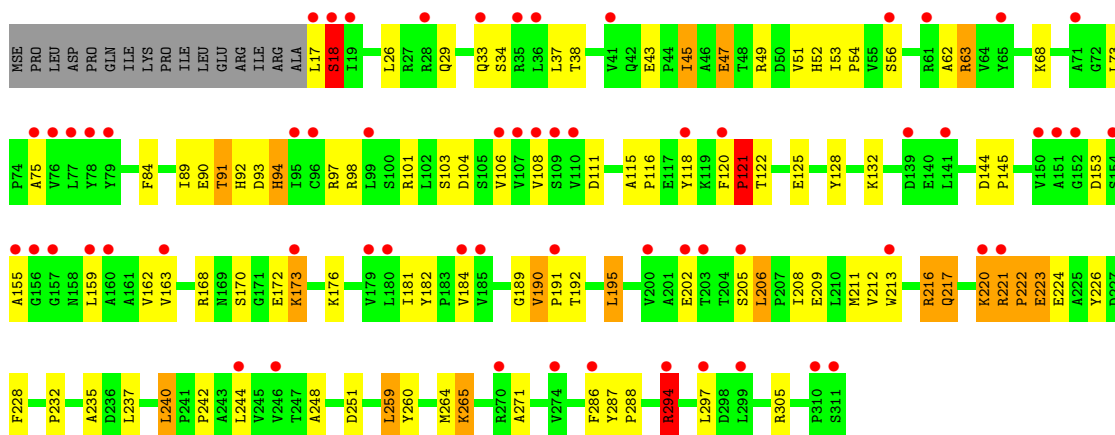
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total	O	0	0
			86	86		
2	B	52	Total	O	0	0
			52	52		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

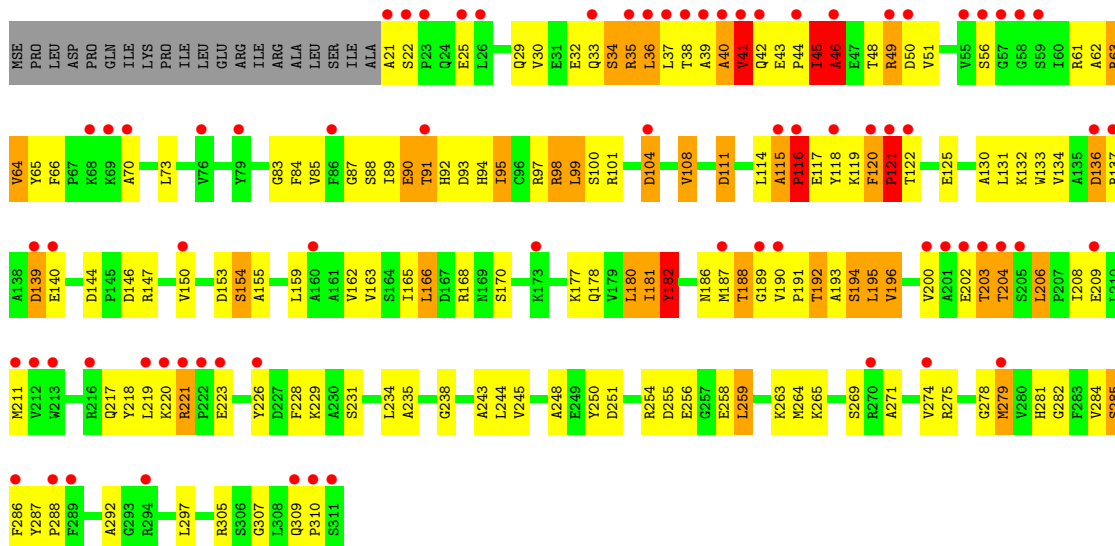
• Molecule 1: CARBOXYLESTERASE

Chain A: 



• Molecule 1: CARBOXYLESTERASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.71Å 73.71Å 234.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 28.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	76.1 (20.00-2.30) 98.5 (28.97-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.261 0.331 , 0.328	Depositor DCC
R_{free} test set	1513 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 10.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 38052 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	4607	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.59	1/2294 (0.0%)	0.95	3/3114 (0.1%)
1	B	0.99	14/2267 (0.6%)	1.48	27/3077 (0.9%)
All	All	0.82	15/4561 (0.3%)	1.25	30/6191 (0.5%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	115	ALA	C-N	21.80	1.75	1.34
1	B	203	THR	C-N	-11.89	1.06	1.34
1	B	114	LEU	C-N	9.98	1.56	1.34
1	B	98	ARG	C-N	-9.69	1.11	1.34
1	B	120	PHE	C-N	7.26	1.48	1.34
1	B	49	ARG	C-N	-5.87	1.20	1.34
1	B	99	LEU	C-N	5.79	1.47	1.34
1	B	258	GLU	C-N	5.73	1.47	1.34
1	B	45	ILE	C-N	-5.70	1.21	1.34
1	B	154	SER	C-N	-5.67	1.21	1.34
1	B	41	VAL	C-N	-5.42	1.21	1.34
1	A	121	PRO	CA-CB	-5.41	1.42	1.53
1	B	279	MSE	CG-SE	-5.37	1.77	1.95
1	B	144	ASP	C-N	-5.36	1.24	1.34
1	B	194	SER	C-N	-5.31	1.21	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	PRO	CA-N-CD	-33.87	64.08	111.50
1	B	121	PRO	CA-N-CD	-32.45	66.07	111.50
1	A	120	PHE	C-N-CD	-23.48	68.93	120.60
1	B	203	THR	O-C-N	-14.45	99.57	122.70
1	A	120	PHE	C-N-CA	13.16	177.27	122.00
1	B	115	ALA	O-C-N	12.53	144.91	121.10
1	B	115	ALA	CA-C-N	-11.95	83.64	117.10
1	B	204	THR	O-C-N	10.44	139.41	122.70
1	B	115	ALA	C-N-CA	10.38	165.61	122.00
1	B	46	ALA	O-C-N	-9.46	107.57	122.70
1	B	203	THR	CA-C-N	8.47	135.84	117.20
1	B	204	THR	CA-C-N	-8.31	98.91	117.20
1	B	116	PRO	N-CA-CB	8.07	112.99	103.30
1	B	46	ALA	CA-C-N	7.69	134.12	117.20
1	B	114	LEU	C-N-CA	-7.40	103.21	121.70
1	B	41	VAL	N-CA-C	-7.33	91.20	111.00
1	B	204	THR	C-N-CA	7.20	139.70	121.70
1	B	45	ILE	C-N-CA	7.15	139.57	121.70
1	B	121	PRO	CA-CB-CG	-6.91	90.88	104.00
1	B	115	ALA	C-N-CD	-6.86	105.50	120.60
1	B	95	ILE	O-C-N	-6.28	112.65	122.70
1	B	94	HIS	O-C-N	6.21	132.64	122.70
1	B	41	VAL	CB-CA-C	-6.08	99.84	111.40
1	B	99	LEU	O-C-N	5.70	131.82	122.70
1	B	45	ILE	CA-C-N	-5.55	104.98	117.20
1	B	120	PHE	C-N-CD	-5.54	108.42	120.60
1	B	182	TYR	CA-CB-CG	5.48	123.81	113.40
1	B	202	GLU	CA-CB-CG	5.44	125.37	113.40
1	A	294	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	116	PRO	CA-CB-CG	-5.08	94.36	104.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	203	THR	Mainchain

5.2 Close contacts ⓘ

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

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2248	0	2251	86	0
1	B	2221	0	2214	146	1
2	A	86	0	0	3	0
2	B	52	0	0	2	0
All	All	4607	0	4465	227	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (227) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:115:ALA:C	1:B:116:PRO:N	1.75	1.37
1:B:243:ALA:HB3	1:B:264:MSE:HE1	1.37	1.07
1:B:115:ALA:CA	1:B:116:PRO:N	2.20	1.03
1:B:264:MSE:HE2	1:B:271:ALA:HB2	1.39	1.02
1:A:265:LYS:HZ1	1:A:271:ALA:N	1.59	1.01
1:B:116:PRO:HD3	1:B:117:GLU:OE2	1.62	0.99
1:B:264:MSE:CE	1:B:271:ALA:HB2	1.92	0.99
1:B:192:THR:HG22	1:B:195:LEU:H	1.26	0.98
1:B:41:VAL:HG22	1:B:43:GLU:HG2	1.46	0.95
1:A:265:LYS:NZ	1:A:271:ALA:H	1.66	0.94
1:B:32:GLU:O	1:B:36:LEU:HB2	1.69	0.93
1:A:260:TYR:HE2	1:A:264:MSE:HE2	1.34	0.92
1:A:68:LYS:HE3	1:A:73:LEU:HD21	1.49	0.92
1:A:29:GLN:HG2	1:A:33:GLN:NE2	1.88	0.88
1:B:104:ASP:HB2	1:B:305:ARG:HH21	1.39	0.87
1:B:50:ASP:OD1	1:B:63:ARG:HD3	1.76	0.85
1:A:260:TYR:CE2	1:A:264:MSE:HE2	2.14	0.82
1:A:29:GLN:HG2	1:A:33:GLN:HE22	1.42	0.82
1:B:120:PHE:CE1	1:B:121:PRO:HD2	2.15	0.81
1:B:42:GLN:O	1:B:44:PRO:HD3	1.80	0.81
1:B:309:GLN:NE2	1:B:309:GLN:HA	1.96	0.79
1:B:120:PHE:O	1:B:121:PRO:HG2	1.81	0.79
1:B:91:THR:HG22	1:B:92:HIS:ND1	1.98	0.78
1:B:118:TYR:HB3	1:B:122:THR:HG21	1.64	0.77
1:A:52:HIS:ND1	2:A:2018:HOH:O	2.11	0.77
1:A:260:TYR:HE2	1:A:264:MSE:CE	1.97	0.77
1:A:91:THR:HG22	1:A:92:HIS:ND1	2.01	0.76
1:B:46:ALA:HB3	1:B:66:PHE:O	1.86	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260:TYR:CE2	1:A:264:MSE:CE	2.69	0.76
1:A:265:LYS:HZ1	1:A:271:ALA:H	0.81	0.75
1:B:192:THR:HG21	1:B:255:ASP:HB2	1.69	0.75
1:B:49:ARG:HB3	1:B:64:VAL:HG13	1.68	0.75
1:B:264:MSE:HE2	1:B:271:ALA:CB	2.15	0.74
1:B:21:ALA:HB1	1:B:25:GLU:CG	2.17	0.73
1:B:41:VAL:CG2	1:B:43:GLU:HG2	2.19	0.73
1:A:265:LYS:NZ	1:A:271:ALA:N	2.31	0.72
1:A:220:LYS:HG3	1:A:221:ARG:N	2.03	0.72
1:B:39:ALA:O	1:B:40:ALA:HB2	1.89	0.71
1:A:189:GLY:O	1:A:191:PRO:HD3	1.90	0.71
1:B:115:ALA:C	1:B:116:PRO:CD	2.60	0.71
1:B:115:ALA:CB	1:B:116:PRO:N	2.55	0.70
1:B:115:ALA:HB1	1:B:116:PRO:N	2.06	0.69
1:B:120:PHE:O	1:B:121:PRO:CG	2.41	0.69
1:B:63:ARG:HG2	1:B:65:TYR:CZ	2.29	0.68
1:A:68:LYS:CE	1:A:73:LEU:HD21	2.22	0.68
1:A:17:LEU:O	1:A:18:SER:HB2	1.93	0.67
1:B:88:SER:OG	1:B:90:GLU:HG2	1.95	0.66
1:B:41:VAL:CG1	1:B:41:VAL:O	2.42	0.66
1:B:208:ILE:HA	1:B:211:MSE:CE	2.26	0.66
1:B:35:ARG:HG2	1:B:36:LEU:N	2.10	0.66
1:B:120:PHE:CD1	1:B:121:PRO:HD2	2.31	0.66
1:A:91:THR:CG2	1:A:92:HIS:ND1	2.59	0.65
1:B:115:ALA:HA	1:B:116:PRO:N	2.11	0.65
1:B:189:GLY:O	1:B:191:PRO:HD3	1.98	0.64
1:A:52:HIS:CE1	2:A:2018:HOH:O	2.50	0.64
1:B:120:PHE:CZ	1:B:121:PRO:HD2	2.32	0.64
1:A:34:SER:O	1:A:37:LEU:HB2	1.97	0.64
1:B:21:ALA:HB1	1:B:25:GLU:CD	2.18	0.64
1:B:85:VAL:HG13	1:B:115:ALA:O	1.98	0.64
1:B:208:ILE:HA	1:B:211:MSE:HE2	1.80	0.64
1:A:51:VAL:CG2	1:A:62:ALA:HB3	2.28	0.63
1:B:104:ASP:HB2	1:B:305:ARG:NH2	2.12	0.63
1:B:95:ILE:HD11	1:B:285:SER:HA	1.81	0.63
1:B:41:VAL:HG13	1:B:41:VAL:O	1.99	0.62
1:B:91:THR:CG2	1:B:92:HIS:ND1	2.62	0.62
1:A:190:VAL:HB	1:B:190:VAL:HG11	1.81	0.62
1:A:172:GLU:C	1:A:173:LYS:HD3	2.20	0.62
1:B:180:LEU:HB2	1:B:245:VAL:HG22	1.82	0.62
1:B:43:GLU:OE2	1:B:287:TYR:OH	2.11	0.61
1:A:190:VAL:HG11	1:B:190:VAL:HB	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:284:VAL:O	1:B:287:TYR:HB3	2.01	0.60
1:A:294:ARG:CG	1:A:294:ARG:HH11	2.14	0.60
1:A:43:GLU:OE1	1:A:101:ARG:NH1	2.34	0.60
1:A:208:ILE:HA	1:A:211:MSE:HE3	1.84	0.59
1:B:133:TRP:HA	1:B:136:ASP:OD1	2.03	0.59
1:A:221:ARG:O	1:A:223:GLU:N	2.36	0.58
1:B:30:VAL:HA	1:B:33:GLN:OE1	2.03	0.58
1:B:21:ALA:HB1	1:B:25:GLU:HG3	1.85	0.58
1:B:279:MSE:SE	1:B:292:ALA:HB3	2.54	0.58
1:B:84:PHE:O	1:B:115:ALA:N	2.37	0.58
1:B:192:THR:HG22	1:B:195:LEU:N	2.08	0.58
1:B:93:ASP:O	1:B:97:ARG:HG3	2.04	0.58
1:A:294:ARG:HH11	1:A:294:ARG:HG3	1.69	0.57
1:B:255:ASP:O	1:B:259:LEU:HD12	2.04	0.57
1:B:265:LYS:HA	1:B:269:SER:O	2.04	0.57
1:A:248:ALA:HB3	1:A:251:ASP:HB2	1.87	0.56
1:B:43:GLU:CD	1:B:287:TYR:HH	2.06	0.56
1:A:121:PRO:O	1:A:125:GLU:HG3	2.06	0.56
1:B:250:TYR:HE2	1:B:278:GLY:HA2	1.70	0.56
1:B:29:GLN:C	1:B:33:GLN:NE2	2.60	0.56
1:B:228:PHE:HB2	1:B:235:ALA:HB2	1.89	0.55
1:B:182:TYR:CE2	1:B:282:GLY:HA2	2.42	0.55
1:A:260:TYR:CE2	1:A:264:MSE:HE3	2.41	0.55
1:A:184:VAL:O	1:A:184:VAL:HG13	2.07	0.55
1:A:192:THR:OG1	1:A:195:LEU:HB2	2.07	0.55
1:A:116:PRO:HB3	1:A:217:GLN:HG3	1.89	0.54
1:A:213:TRP:HA	1:A:216:ARG:HG3	1.89	0.54
1:B:243:ALA:HB3	1:B:264:MSE:CE	2.26	0.54
1:A:51:VAL:HG22	1:A:62:ALA:HB3	1.89	0.53
1:B:39:ALA:O	1:B:40:ALA:CB	2.53	0.53
1:B:51:VAL:HG23	1:B:62:ALA:HB3	1.90	0.53
1:A:259:LEU:HD21	1:B:193:ALA:HA	1.90	0.53
1:B:248:ALA:HB3	1:B:251:ASP:HB2	1.91	0.53
1:A:29:GLN:CG	1:A:33:GLN:NE2	2.69	0.53
1:B:49:ARG:HB3	1:B:64:VAL:CG1	2.37	0.52
1:A:294:ARG:HH11	1:A:294:ARG:CB	2.21	0.52
1:A:294:ARG:CZ	2:A:2082:HOH:O	2.58	0.52
1:A:260:TYR:CD2	1:A:264:MSE:HE3	2.44	0.52
1:B:45:ILE:HD11	1:B:100:SER:HB3	1.91	0.52
1:A:89:ILE:HD11	1:A:111:ASP:HB2	1.92	0.52
1:B:286:PHE:C	1:B:288:PRO:HD2	2.30	0.52
1:B:43:GLU:OE1	1:B:101:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:43:GLU:OE2	1:B:98:ARG:HD2	2.09	0.52
1:A:221:ARG:O	1:A:224:GLU:HG3	2.10	0.51
1:B:21:ALA:HB1	1:B:25:GLU:OE2	2.09	0.51
1:A:168:ARG:HD3	1:A:240:LEU:HD13	1.90	0.51
1:B:162:VAL:HG12	1:B:166:LEU:HD22	1.91	0.51
1:A:29:GLN:CG	1:A:33:GLN:HE22	2.18	0.51
1:A:173:LYS:HD3	1:A:173:LYS:N	2.26	0.51
1:B:192:THR:CG2	1:B:255:ASP:HB2	2.37	0.50
1:B:256:GLU:HG2	2:B:2041:HOH:O	2.11	0.50
1:B:120:PHE:O	1:B:121:PRO:CB	2.59	0.50
1:B:131:LEU:HD22	1:B:163:VAL:CG1	2.42	0.50
1:A:265:LYS:NZ	1:A:265:LYS:HB2	2.26	0.50
1:B:187:MSE:HE1	1:B:218:TYR:HD2	1.76	0.50
1:B:186:ASN:ND2	1:B:188:THR:H	2.10	0.50
1:A:206:LEU:HD22	1:A:211:MSE:CG	2.42	0.50
1:B:279:MSE:HE2	1:B:279:MSE:HA	1.94	0.50
1:A:45:ILE:HG23	1:A:47:GLU:H	1.76	0.50
1:B:108:VAL:HG11	1:B:134:VAL:HG21	1.94	0.49
1:B:87:GLY:HA2	1:B:91:THR:HG21	1.93	0.49
1:B:147:ARG:NH2	1:B:310:PRO:HD3	2.27	0.49
1:A:162:VAL:HG22	1:A:232:PRO:HG3	1.94	0.49
1:B:120:PHE:CD1	1:B:121:PRO:CD	2.95	0.49
1:B:83:GLY:O	1:B:84:PHE:HB2	2.13	0.48
1:A:206:LEU:HD22	1:A:211:MSE:HG3	1.95	0.48
1:B:29:GLN:O	1:B:33:GLN:CD	2.51	0.48
1:B:231:SER:HB2	1:B:234:LEU:HD12	1.96	0.48
1:B:89:ILE:HG13	1:B:111:ASP:OD2	2.14	0.48
1:A:191:PRO:HG2	1:B:259:LEU:HD22	1.96	0.48
1:A:128:TYR:CE2	1:A:132:LYS:HE3	2.49	0.47
1:B:90:GLU:CD	1:B:90:GLU:H	2.16	0.47
1:A:93:ASP:O	1:A:97:ARG:HG3	2.13	0.47
1:B:177:LYS:HD3	1:B:307:GLY:HA3	1.97	0.47
1:B:154:SER:HA	1:B:182:TYR:O	2.14	0.47
1:B:250:TYR:CE2	1:B:278:GLY:HA2	2.49	0.47
1:B:51:VAL:CG2	1:B:62:ALA:HB3	2.44	0.47
1:B:116:PRO:HB3	1:B:217:GLN:OE1	2.14	0.47
1:B:70:ALA:HB3	1:B:73:LEU:HD21	1.96	0.47
1:B:108:VAL:HG22	1:B:108:VAL:O	2.15	0.47
1:B:209:GLU:CD	1:B:209:GLU:H	2.15	0.47
1:B:264:MSE:HE3	1:B:271:ALA:HB2	1.89	0.46
1:A:176:LYS:O	1:A:242:PRO:HD2	2.16	0.46
1:B:208:ILE:HA	1:B:211:MSE:HE3	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:103:SER:O	1:A:104:ASP:HB2	2.15	0.46
1:A:221:ARG:HA	1:A:222:PRO:HD2	1.68	0.46
1:B:243:ALA:CB	1:B:264:MSE:HE1	2.25	0.46
1:B:119:LYS:HD2	1:B:220:LYS:HD3	1.98	0.46
1:B:120:PHE:O	1:B:121:PRO:HB2	2.16	0.46
1:B:61:ARG:NH1	1:B:90:GLU:OE1	2.45	0.45
1:A:89:ILE:HG13	1:A:111:ASP:OD1	2.15	0.45
1:B:196:VAL:O	1:B:200:VAL:HG23	2.17	0.45
1:A:115:ALA:HB1	1:A:217:GLN:O	2.17	0.45
1:B:235:ALA:O	1:B:263:LYS:NZ	2.49	0.45
1:A:294:ARG:NH1	1:A:294:ARG:HG3	2.32	0.45
1:B:130:ALA:O	1:B:131:LEU:C	2.55	0.45
1:A:153:ASP:HA	1:A:181:ILE:O	2.17	0.45
1:A:94:HIS:ND1	1:A:94:HIS:N	2.65	0.45
1:A:98:ARG:HG3	1:A:98:ARG:HH11	1.81	0.45
1:B:150:VAL:O	1:B:150:VAL:HG23	2.17	0.45
1:A:189:GLY:O	1:A:191:PRO:CD	2.64	0.44
1:A:17:LEU:O	1:A:18:SER:CB	2.65	0.44
1:B:177:LYS:HG3	1:B:178:GLN:N	2.32	0.44
1:B:43:GLU:HG3	1:B:287:TYR:OH	2.18	0.44
1:B:165:ILE:HG23	1:B:168:ARG:NH2	2.32	0.44
1:A:98:ARG:HG3	1:A:98:ARG:NH1	2.33	0.44
1:A:75:ALA:HA	1:A:106:VAL:O	2.18	0.44
1:B:153:ASP:HA	1:B:181:ILE:O	2.17	0.44
1:B:309:GLN:HE21	1:B:309:GLN:HA	1.78	0.44
1:A:118:TYR:HB3	1:A:122:THR:HG21	1.99	0.44
1:A:226:TYR:CE2	1:B:226:TYR:CE2	3.05	0.44
1:B:192:THR:HB	1:B:195:LEU:HB2	2.00	0.44
1:B:120:PHE:CD1	1:B:121:PRO:N	2.86	0.44
1:B:133:TRP:NE1	1:B:137:ARG:HD3	2.33	0.43
1:A:212:VAL:O	1:A:216:ARG:HG2	2.17	0.43
1:A:170:SER:OG	1:A:172:GLU:HG3	2.17	0.43
1:B:284:VAL:HG13	1:B:297:LEU:HG	2.01	0.43
1:B:137:ARG:O	1:B:140:GLU:HB2	2.18	0.43
1:B:104:ASP:CB	1:B:305:ARG:HH21	2.21	0.43
1:A:159:LEU:O	1:A:163:VAL:HG23	2.18	0.43
1:B:206:LEU:HG	1:B:281:HIS:CD2	2.54	0.43
1:B:287:TYR:CD1	1:B:288:PRO:N	2.87	0.43
1:A:237:LEU:HA	1:A:240:LEU:CD2	2.48	0.43
1:A:63:ARG:NH2	1:A:90:GLU:OE1	2.46	0.42
1:B:192:THR:HG23	1:B:193:ALA:N	2.34	0.42
1:B:166:LEU:HA	1:B:166:LEU:HD12	1.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:LYS:HZ3	1:A:271:ALA:HB3	1.84	0.42
1:A:121:PRO:HD2	1:A:122:THR:H	1.84	0.42
1:B:178:GLN:CG	1:B:243:ALA:HB2	2.49	0.42
1:A:228:PHE:HB2	1:A:235:ALA:HB2	2.02	0.42
1:B:309:GLN:CA	1:B:309:GLN:NE2	2.67	0.42
1:B:22:SER:O	1:B:25:GLU:HG2	2.20	0.42
1:B:155:ALA:O	1:B:159:LEU:HG	2.19	0.42
1:B:41:VAL:CG2	1:B:43:GLU:CG	2.95	0.41
1:B:34:SER:O	1:B:38:THR:HG23	2.20	0.41
1:A:63:ARG:HB2	1:A:89:ILE:HG21	2.01	0.41
1:B:33:GLN:O	1:B:37:LEU:HG	2.19	0.41
1:A:53:ILE:HA	1:A:54:PRO:HD3	1.88	0.41
1:B:121:PRO:O	1:B:125:GLU:N	2.51	0.41
1:B:48:THR:HA	1:B:64:VAL:O	2.19	0.41
1:A:162:VAL:CG2	1:A:232:PRO:HG3	2.50	0.41
1:A:84:PHE:CE1	1:A:155:ALA:HB1	2.55	0.41
1:B:309:GLN:CA	1:B:309:GLN:HE21	2.33	0.41
1:B:285:SER:HB2	2:B:2024:HOH:O	2.21	0.41
1:B:29:GLN:O	1:B:33:GLN:NE2	2.54	0.41
1:B:162:VAL:HG21	1:B:229:LYS:O	2.21	0.41
1:A:38:THR:HG22	1:A:94:HIS:ND1	2.36	0.41
1:B:168:ARG:NH1	1:B:238:GLY:O	2.50	0.41
1:B:192:THR:CG2	1:B:193:ALA:N	2.84	0.40
1:A:144:ASP:HA	1:A:145:PRO:HD2	1.84	0.40
1:A:286:PHE:C	1:A:288:PRO:CD	2.90	0.40
1:B:63:ARG:HG2	1:B:65:TYR:CE2	2.56	0.40
1:B:61:ARG:HG2	1:B:89:ILE:HD12	2.03	0.40
1:B:45:ILE:CD1	1:B:100:SER:HB3	2.50	0.40
1:B:254:ARG:HD2	1:B:275:ARG:NE	2.37	0.40
1:B:192:THR:HG22	1:B:194:SER:N	2.36	0.40
1:A:26:LEU:HD12	1:A:26:LEU:HA	1.81	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:B:139:ASP:N	1:B:221:ARG:NH2[6_455]	1.63	0.57

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 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	293/311 (94%)	280 (96%)	9 (3%)	4 (1%)	16	15
1	B	289/311 (93%)	262 (91%)	21 (7%)	6 (2%)	11	8
All	All	582/622 (94%)	542 (93%)	30 (5%)	10 (2%)	14	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PRO
1	A	222	PRO
1	B	40	ALA
1	B	41	VAL
1	B	46	ALA
1	B	116	PRO
1	B	121	PRO
1	A	18	SER
1	B	188	THR
1	A	190	VAL

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 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	233/244 (96%)	204 (88%)	29 (12%)	7	7
1	B	230/244 (94%)	195 (85%)	35 (15%)	4	4
All	All	463/488 (95%)	399 (86%)	64 (14%)	5	5

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	45	ILE
1	A	47	GLU
1	A	49	ARG
1	A	56	SER
1	A	63	ARG
1	A	91	THR
1	A	94	HIS
1	A	108	VAL
1	A	173	LYS
1	A	182	TYR
1	A	195	LEU
1	A	202	GLU
1	A	205	SER
1	A	206	LEU
1	A	209	GLU
1	A	216	ARG
1	A	217	GLN
1	A	220	LYS
1	A	221	ARG
1	A	223	GLU
1	A	240	LEU
1	A	244	LEU
1	A	259	LEU
1	A	265	LYS
1	A	287	TYR
1	A	294	ARG
1	A	297	LEU
1	A	305	ARG
1	B	34	SER
1	B	35	ARG
1	B	36	LEU
1	B	45	ILE
1	B	56	SER
1	B	63	ARG
1	B	64	VAL
1	B	90	GLU
1	B	91	THR
1	B	99	LEU
1	B	104	ASP
1	B	108	VAL
1	B	111	ASP
1	B	121	PRO

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Mol	Chain	Res	Type
1	B	132	LYS
1	B	136	ASP
1	B	139	ASP
1	B	146	ASP
1	B	166	LEU
1	B	170	SER
1	B	180	LEU
1	B	181	ILE
1	B	182	TYR
1	B	192	THR
1	B	195	LEU
1	B	196	VAL
1	B	204	THR
1	B	206	LEU
1	B	219	LEU
1	B	221	ARG
1	B	223	GLU
1	B	244	LEU
1	B	259	LEU
1	B	274	VAL
1	B	285	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	33	GLN
1	A	309	GLN
1	B	186	ASN
1	B	309	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/311 (94%)	1.45	62 (21%) ⓘ ⓘ	6, 16, 32, 42	3 (1%)
1	B	291/311 (93%)	1.46	74 (25%) ⓘ ⓘ	0, 0, 0, 0	0
All	All	586/622 (94%)	1.45	136 (23%) ⓘ ⓘ	0, 7, 28, 42	3 (0%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	SER	9.9
1	B	41	VAL	6.8
1	B	121	PRO	5.6
1	B	310	PRO	5.6
1	B	33	GLN	5.6
1	B	221	ARG	5.5
1	B	21	ALA	5.0
1	B	203	THR	4.9
1	B	26	LEU	4.8
1	B	202	GLU	4.6
1	B	37	LEU	4.6
1	B	39	ALA	4.6
1	B	204	THR	4.6
1	B	36	LEU	4.4
1	A	202	GLU	4.4
1	B	289	PHE	4.2
1	A	33	GLN	4.2
1	B	189	GLY	4.1
1	B	25	GLU	4.1
1	B	139	ASP	4.1
1	A	203	THR	4.0
1	B	68	LYS	4.0
1	B	22	SER	3.9
1	B	40	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	17	LEU	3.9
1	B	58	GLY	3.8
1	A	151	ALA	3.8
1	B	35	ARG	3.8
1	B	222	PRO	3.7
1	B	216	ARG	3.6
1	A	160	ALA	3.5
1	B	140	GLU	3.5
1	B	69	LYS	3.5
1	A	79	TYR	3.5
1	B	42	GLN	3.5
1	A	18	SER	3.5
1	B	56	SER	3.5
1	A	107	VAL	3.5
1	B	136	ASP	3.4
1	B	137	ARG	3.4
1	B	86	PHE	3.4
1	B	200	VAL	3.4
1	A	76	VAL	3.3
1	A	108	VAL	3.3
1	B	38	THR	3.2
1	A	150	VAL	3.2
1	B	219	LEU	3.1
1	B	118	TYR	3.1
1	A	246	VAL	3.0
1	A	184	VAL	3.0
1	A	71	ALA	3.0
1	A	220	LYS	3.0
1	A	286	PHE	3.0
1	A	179	VAL	2.9
1	A	78	TYR	2.9
1	B	115	ALA	2.9
1	A	141	LEU	2.9
1	A	270	ARG	2.9
1	B	223	GLU	2.8
1	A	155	ALA	2.8
1	B	311	SER	2.8
1	B	116	PRO	2.8
1	B	294	ARG	2.8
1	A	152	GLY	2.8
1	B	59	SER	2.8
1	A	41	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	2.8
1	B	44	PRO	2.7
1	A	191	PRO	2.7
1	B	286	PHE	2.7
1	A	163	VAL	2.7
1	B	46	ALA	2.7
1	A	36	LEU	2.6
1	A	99	LEU	2.6
1	B	23	PRO	2.6
1	A	200	VAL	2.6
1	A	61	ARG	2.6
1	B	209	GLU	2.6
1	A	28	ARG	2.6
1	B	187	MSE	2.6
1	A	221	ARG	2.5
1	B	205	SER	2.5
1	A	19	ILE	2.5
1	B	120	PHE	2.5
1	B	49	ARG	2.5
1	B	213	TRP	2.5
1	B	212	VAL	2.5
1	A	299	LEU	2.4
1	A	205	SER	2.4
1	A	310	PRO	2.4
1	B	190	VAL	2.4
1	A	109	SER	2.4
1	A	157	GLY	2.4
1	A	56	SER	2.4
1	B	226	TYR	2.4
1	B	309	GLN	2.4
1	B	270	ARG	2.4
1	A	274	VAL	2.3
1	A	95	ILE	2.3
1	B	76	VAL	2.3
1	B	150	VAL	2.3
1	A	96	CYS	2.3
1	A	173	LYS	2.3
1	B	57	GLY	2.3
1	B	288	PRO	2.3
1	A	120	PHE	2.3
1	B	55	VAL	2.3
1	B	274	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	294	ARG	2.2
1	A	139	ASP	2.2
1	A	159	LEU	2.2
1	B	70	ALA	2.2
1	B	91	THR	2.2
1	A	75	ALA	2.2
1	A	77	LEU	2.2
1	A	297	LEU	2.2
1	B	160	ALA	2.2
1	A	180	LEU	2.2
1	B	220	LYS	2.2
1	A	65	TYR	2.2
1	B	201	ALA	2.2
1	A	110	VAL	2.2
1	B	279	MSE	2.1
1	A	35	ARG	2.1
1	B	79	TYR	2.1
1	B	173	LYS	2.1
1	A	106	VAL	2.1
1	A	118	TYR	2.1
1	A	154	SER	2.1
1	A	185	VAL	2.1
1	B	50	ASP	2.1
1	A	213	TRP	2.1
1	B	104	ASP	2.1
1	B	122	THR	2.1
1	A	156	GLY	2.0
1	B	211	MSE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.