



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:36 AM UTC

PDB ID : 2C7B / pdb_00002c7b
Title : The Crystal Structure of EstE1, a New Thermophilic and Thermostable Carboxylesterase Cloned from a Metagenomic Library
Authors : Byun, J.-S.; Rhee, J.-K.; Kim, D.-U.; Oh, J.-W.; Cho, H.-S.
Deposited on : 2005-11-21
Resolution : 2.30 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

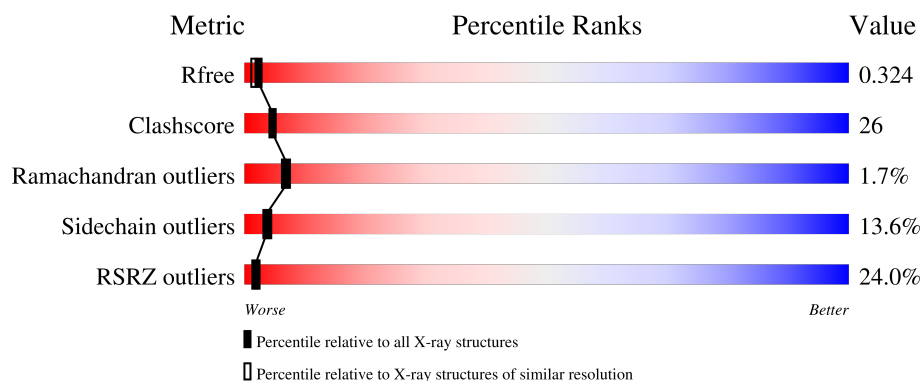
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 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 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			

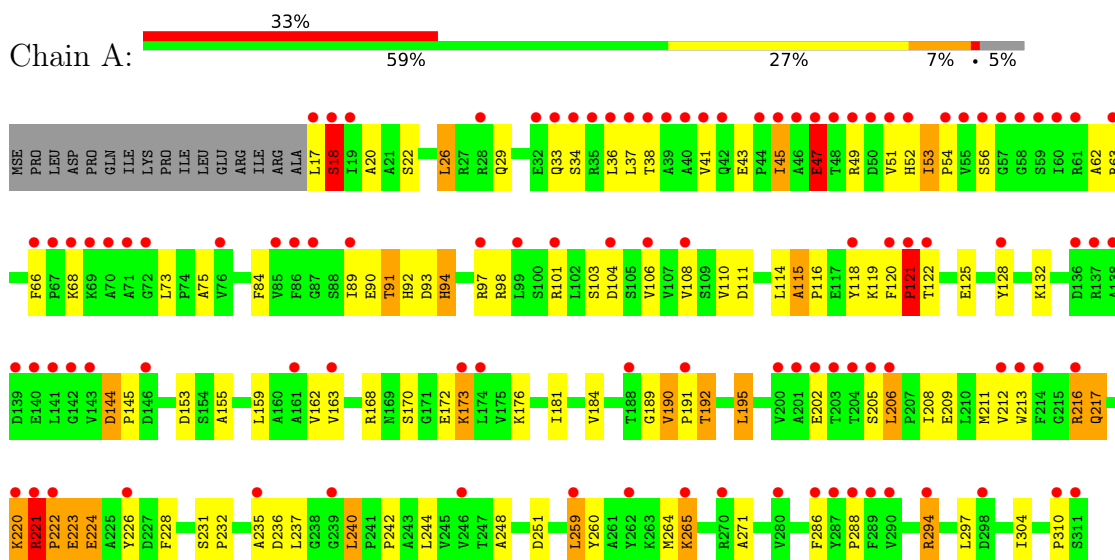
- Molecule 2 is water.

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

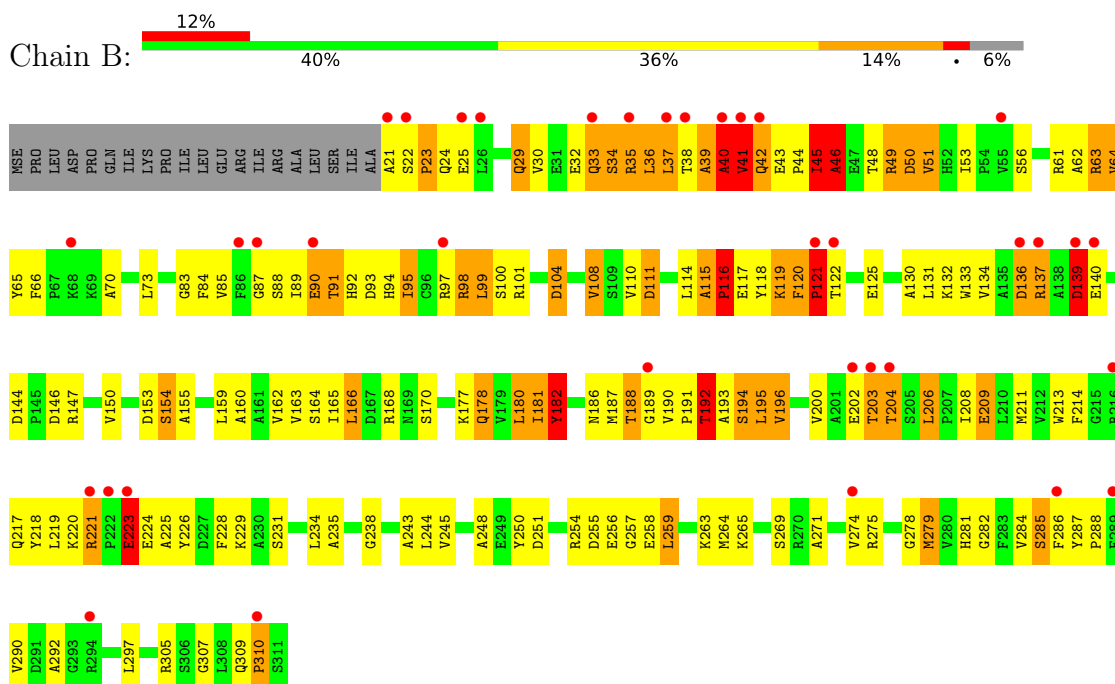
3 Residue-property plots

These plots are drawn for all protein, RNA, 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 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



• Molecule 1: CARBOXYLESTERASE



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 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	76.1 (20.00-2.30) 99.2 (20.00-2.30)	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 0.329 , 0.324	Depositor DCC
R_{free} test set	1907 reflections (5.01%)	wwPDB-VP
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 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.76	3/2294 (0.1%)	1.70	27/3114 (0.9%)
1	B	1.42	27/2267 (1.2%)	2.14	68/3077 (2.2%)
All	All	1.13	30/4561 (0.7%)	1.93	95/6191 (1.5%)

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 (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	THR	C-N	-20.41	1.06	1.33
1	B	115	ALA	C-N	17.88	1.75	1.33
1	B	98	ARG	C-N	-17.39	1.11	1.33
1	B	114	LEU	C-N	16.39	1.56	1.33
1	B	99	LEU	C-N	10.77	1.47	1.33
1	B	258	GLU	C-N	9.62	1.47	1.34
1	B	154	SER	C-N	-9.57	1.21	1.33
1	B	194	SER	C-N	-9.48	1.21	1.33
1	B	41	VAL	C-N	-9.18	1.21	1.33
1	B	50	ASP	C-N	9.18	1.44	1.33
1	B	49	ARG	C-N	-9.10	1.20	1.33
1	B	45	ILE	C-N	-9.10	1.21	1.33
1	B	121	PRO	C-N	8.47	1.45	1.33
1	A	121	PRO	CA-CB	-7.78	1.42	1.53
1	B	42	GLN	N-CA	-7.47	1.37	1.46
1	B	144	ASP	C-N	-7.29	1.24	1.34
1	B	192	THR	C-N	6.97	1.43	1.33
1	B	160	ALA	C-N	6.93	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	42	GLN	CA-C	-6.68	1.45	1.53
1	B	279	MSE	SE-CE	-6.27	1.76	1.95
1	B	279	MSE	CG-SE	-6.08	1.77	1.95
1	B	120	PHE	C-N	6.07	1.48	1.33
1	B	41	VAL	CA-C	-5.74	1.45	1.52
1	A	310	PRO	C-N	-5.55	1.25	1.33
1	B	94	HIS	C-N	5.54	1.40	1.33
1	A	120	PHE	C-O	5.50	1.31	1.24
1	B	202	GLU	CA-CB	5.37	1.62	1.53
1	B	310	PRO	C-N	-5.22	1.26	1.33
1	B	23	PRO	N-CA	-5.16	1.40	1.47
1	B	37	LEU	CA-C	5.01	1.59	1.52

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	PHE	CA-C-N	45.94	177.27	119.84
1	A	120	PHE	C-N-CA	45.94	177.27	119.84
1	B	115	ALA	CA-C-N	36.61	165.61	119.84
1	B	115	ALA	C-N-CA	36.61	165.61	119.84
1	B	116	PRO	CA-N-CD	-34.23	64.08	112.00
1	B	121	PRO	CA-N-CD	-32.81	66.07	112.00
1	B	203	THR	O-C-N	-19.55	99.57	122.05
1	B	115	ALA	O-C-N	16.75	144.91	121.12
1	B	204	THR	O-C-N	14.58	139.41	122.79
1	A	120	PHE	C-N-CD	-13.68	68.93	125.00
1	B	114	LEU	CA-C-N	-11.70	103.21	121.92
1	B	114	LEU	C-N-CA	-11.70	103.21	121.92
1	B	46	ALA	O-C-N	-11.30	107.57	122.59
1	B	204	THR	CA-C-N	10.66	139.70	122.65
1	B	204	THR	C-N-CA	10.66	139.70	122.65
1	B	42	GLN	OE1-CD-NE2	-10.12	112.47	122.60
1	B	33	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	B	178	GLN	OE1-CD-NE2	-9.54	113.06	122.60
1	B	29	GLN	OE1-CD-NE2	-9.46	113.14	122.60
1	B	95	ILE	O-C-N	-9.45	112.65	121.91
1	B	45	ILE	CA-C-N	9.44	139.57	121.54
1	B	45	ILE	C-N-CA	9.44	139.57	121.54
1	B	116	PRO	N-CA-CB	9.27	112.99	103.25
1	B	94	HIS	O-C-N	9.20	132.64	122.15
1	B	144	ASP	CA-C-N	9.16	129.22	119.05
1	B	144	ASP	C-N-CA	9.16	129.22	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	GLN	OE1-CD-NE2	-9.12	113.48	122.60
1	B	99	LEU	O-C-N	9.07	131.82	122.03
1	B	95	ILE	CA-C-N	8.97	133.20	120.28
1	B	95	ILE	C-N-CA	8.97	133.20	120.28
1	B	41	VAL	CA-C-N	-8.88	110.17	122.95
1	B	41	VAL	C-N-CA	-8.88	110.17	122.95
1	B	115	ALA	N-CA-C	8.81	122.93	110.07
1	A	224	GLU	N-CA-C	-8.72	102.08	112.89
1	B	41	VAL	N-CA-C	-8.72	91.20	109.34
1	A	36	LEU	N-CA-C	-8.40	102.08	111.82
1	A	221	ARG	CA-C-N	7.99	129.83	119.84
1	A	221	ARG	C-N-CA	7.99	129.83	119.84
1	A	66	PHE	CA-C-N	7.68	127.23	118.85
1	A	66	PHE	C-N-CA	7.68	127.23	118.85
1	A	20	ALA	N-CA-C	-7.53	103.05	111.71
1	B	144	ASP	O-C-N	-7.39	115.02	121.31
1	B	51	VAL	O-C-N	7.33	130.67	122.97
1	B	110	VAL	N-CA-C	7.22	118.27	107.80
1	B	121	PRO	CA-CB-CG	-7.17	90.88	104.50
1	B	29	GLN	CG-CD-NE2	7.12	127.08	116.40
1	B	42	GLN	CG-CD-NE2	7.04	126.97	116.40
1	B	41	VAL	CB-CA-C	-6.98	99.84	111.29
1	B	257	GLY	O-C-N	-6.97	115.49	122.18
1	A	144	ASP	CA-C-N	6.92	127.50	119.47
1	A	144	ASP	C-N-CA	6.92	127.50	119.47
1	A	22	SER	CA-C-N	6.76	126.55	119.05
1	A	22	SER	C-N-CA	6.76	126.55	119.05
1	A	236	ASP	N-CA-C	-6.60	98.46	108.96
1	B	33	GLN	CG-CD-NE2	6.58	126.26	116.40
1	B	24	GLN	CG-CD-NE2	6.54	126.21	116.40
1	B	94	HIS	CA-C-N	-6.54	112.32	120.56
1	B	94	HIS	C-N-CA	-6.54	112.32	120.56
1	B	114	LEU	N-CA-C	6.40	119.89	109.59
1	B	257	GLY	CA-C-N	6.32	129.92	120.31
1	B	257	GLY	C-N-CA	6.32	129.92	120.31
1	B	51	VAL	CA-C-N	-6.21	113.17	122.74
1	B	51	VAL	C-N-CA	-6.21	113.17	122.74
1	B	178	GLN	CG-CD-NE2	6.14	125.62	116.40
1	B	137	ARG	CB-CA-C	-6.13	101.25	111.13
1	B	39	ALA	N-CA-C	-6.03	103.12	111.81
1	B	139	ASP	N-CA-C	-6.03	104.62	111.07
1	A	26	LEU	N-CA-C	-6.02	104.84	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ALA	CA-C-N	5.92	132.63	121.97
1	B	40	ALA	C-N-CA	5.92	132.63	121.97
1	A	231	SER	CA-C-N	5.90	126.31	119.47
1	A	231	SER	C-N-CA	5.90	126.31	119.47
1	A	110	VAL	N-CA-C	5.84	116.71	108.36
1	A	114	LEU	N-CA-C	5.83	119.46	110.42
1	A	192	THR	N-CA-C	-5.83	100.89	109.81
1	B	116	PRO	CB-CA-C	5.70	120.97	111.56
1	B	203	THR	CA-C-N	5.68	131.32	120.97
1	B	203	THR	C-N-CA	5.68	131.32	120.97
1	B	224	GLU	N-CA-C	-5.68	105.18	111.71
1	B	164	SER	CA-C-N	-5.67	112.45	121.02
1	B	164	SER	C-N-CA	-5.67	112.45	121.02
1	B	202	GLU	CA-CB-CG	5.64	125.37	114.10
1	B	115	ALA	CA-C-O	5.63	129.38	121.27
1	B	53	ILE	N-CA-C	5.62	114.14	107.73
1	A	119	LYS	N-CA-C	5.52	118.59	110.59
1	B	182	TYR	CA-CB-CG	5.51	123.81	113.90
1	B	116	PRO	CB-CG-CD	-5.51	88.48	106.10
1	A	53	ILE	N-CA-C	5.42	114.44	108.05
1	B	116	PRO	CA-CB-CG	-5.34	94.36	104.50
1	A	115	ALA	N-CA-C	-5.33	103.22	110.36
1	A	41	VAL	N-CA-C	5.13	115.87	108.48
1	A	47	GLU	N-CA-C	5.11	116.28	108.42
1	B	223	GLU	N-CA-C	-5.07	107.10	113.28
1	A	120	PHE	O-C-N	5.04	127.11	121.32
1	B	119	LYS	N-CA-C	5.02	117.01	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	203	THR	Mainchain

5.2 Too-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 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	2248	0	2251	87	0
1	B	2221	0	2215	149	1
2	A	86	0	0	3	0
2	B	52	0	0	2	0
All	All	4607	0	4466	231	1

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 26.

All (231) 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:115:ALA:C	1:B:116:PRO:N	1.75	1.42
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:HA	1:B:309:GLN:NE2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ALA:C	1:B:116:PRO:CD	2.60	0.75
1:B:49:ARG:HB3	1:B:64:VAL:HG13	1.68	0.75
1:B:192:THR:HG21	1:B:255:ASP:HB2	1.69	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:A:189:GLY:O	1:A:191:PRO:HD3	1.90	0.71
1:B:39:ALA:O	1:B:40:ALA:HB2	1.89	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:21:ALA:HB1	1:B:25:GLU:CD	2.18	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:A:172:GLU:C	1:A:173:LYS:HD3	2.20	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:B:43:GLU:OE2	1:B:287:TYR:OH	2.11	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: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:O	1:B:41:VAL:HG13	1.99	0.62
1:A:190:VAL:HB	1:B:190:VAL:HG11	1.81	0.62
1:B:91:THR:CG2	1:B:92:HIS:ND1	2.62	0.62
1:B:180:LEU:HB2	1:B:245:VAL:HG22	1.82	0.62
1:A:190:VAL:HG11	1:B:190:VAL:HB	1.83	0.61
1:B:284:VAL:O	1:B:287:TYR:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:HH11	1:A:294:ARG:CG	2.14	0.60
1:B:29:GLN:C	1:B:33:GLN:NE2	2.60	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:93:ASP:O	1:B:97:ARG:HG3	2.04	0.58
1:B:192:THR:HG22	1:B:195:LEU:N	2.08	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:B:286:PHE:C	1:B:288:PRO:HD2	2.30	0.56
1:A:248:ALA:HB3	1:A:251:ASP:HB2	1.87	0.56
1:B:43:GLU:CD	1:B:287:TYR:HH	2.11	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:182:TYR:CE2	1:B:282:GLY:HA2	2.42	0.55
1:B:228:PHE:HB2	1:B:235:ALA:HB2	1.89	0.55
1:A:260:TYR:CE2	1:A:264:MSE:HE3	2.41	0.55
1:A:184:VAL:HG13	1:A:184:VAL:O	2.07	0.55
1:A:192:THR:OG1	1:A:195:LEU:HB2	2.07	0.55
1:B:209:GLU:H	1:B:209:GLU:CD	2.15	0.54
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:B:29:GLN:O	1:B:33:GLN:CD	2.51	0.53
1:A:29:GLN:CG	1:A:33:GLN:NE2	2.69	0.53
1:A:294:ARG:HH11	1:A:294:ARG:CB	2.21	0.52
1:B:49:ARG:HB3	1:B:64:VAL:CG1	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HD11	1:A:111:ASP:HB2	1.92	0.52
1:B:43:GLU:OE1	1:B:101:ARG:NH2	2.43	0.52
1:B:43:GLU:OE2	1:B:98:ARG:HD2	2.09	0.52
1:B:90:GLU:CD	1:B:90:GLU:H	2.16	0.51
1:A:221:ARG:O	1:A:224:GLU:HG3	2.10	0.51
1:A:168:ARG:HD3	1:A:240:LEU:HD13	1.90	0.51
1:B:21:ALA:HB1	1:B:25:GLU:OE2	2.09	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:186:ASN:ND2	1:B:188:THR:H	2.10	0.50
1:B:187:MSE:HE1	1:B:218:TYR:HD2	1.76	0.50
1:A:45:ILE:HG23	1:A:47:GLU:H	1.76	0.50
1:A:206:LEU:HD22	1:A:211:MSE:CG	2.42	0.50
1:B:130:ALA:O	1:B:131:LEU:C	2.55	0.50
1:B:279:MSE:HE2	1:B:279:MSE:HA	1.94	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: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: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:51:VAL:CG2	1:B:62:ALA:HB3	2.44	0.47
1:B:250:TYR:CE2	1:B:278:GLY:HA2	2.49	0.47
1:B:70:ALA:HB3	1:B:73:LEU:HD21	1.96	0.47
1:B:116:PRO:HB3	1:B:217:GLN:OE1	2.14	0.47
1:B:108:VAL:O	1:B:108:VAL:HG22	2.15	0.47
1:A:176:LYS:O	1:A:242:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:MSE:HE3	1:B:271:ALA:HB2	1.89	0.46
1:A:103:SER:O	1:A:104:ASP:HB2	2.15	0.46
1:B:208:ILE:HA	1:B:211:MSE:HE3	1.98	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:A:89:ILE:HG13	1:A:111:ASP:OD1	2.15	0.45
1:B:61:ARG:NH1	1:B:90:GLU:OE1	2.45	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:286:PHE:C	1:A:288:PRO:CD	2.90	0.45
1:A:294:ARG:HG3	1:A:294:ARG:NH1	2.32	0.45
1:A:94:HIS:ND1	1:A:94:HIS:N	2.65	0.45
1:A:153:ASP:HA	1:A:181:ILE:O	2.17	0.45
1:A:98:ARG:HG3	1:A:98:ARG:HH11	1.81	0.45
1:B:150:VAL:HG23	1:B:150:VAL:O	2.17	0.45
1:A:17:LEU:O	1:A:18:SER:CB	2.65	0.44
1:A:189:GLY:O	1:A:191:PRO:CD	2.64	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:75:ALA:HA	1:A:106:VAL:O	2.18	0.44
1:A:98:ARG:HG3	1:A:98:ARG:NH1	2.33	0.44
1:B:153:ASP:HA	1:B:181:ILE:O	2.17	0.44
1:B:177:LYS:HG3	1:B:178:GLN:N	2.32	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:309:GLN:HA	1:B:309:GLN:HE21	1.78	0.44
1:B:120:PHE:CD1	1:B:121:PRO:N	2.86	0.44
1:B:192:THR:HB	1:B:195:LEU:HB2	2.00	0.44
1:A:212:VAL:O	1:A:216:ARG:HG2	2.17	0.43
1:B:133:TRP:NE1	1:B:137:ARG:HD3	2.33	0.43
1:B:213:TRP:O	1:B:214:PHE:C	2.61	0.43
1:A:170:SER:OG	1:A:172:GLU:HG3	2.17	0.43
1:B:22:SER:O	1:B:23:PRO:C	2.61	0.43
1:B:137:ARG:O	1:B:140:GLU:HB2	2.18	0.43
1:B:284:VAL:HG13	1:B:297:LEU:HG	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:HA	1:A:240:LEU:CD2	2.48	0.43
1:B:287:TYR:CD1	1:B:288:PRO:N	2.87	0.43
1:A:63:ARG:NH2	1:A:90:GLU:OE1	2.46	0.42
1:B:166:LEU:HD12	1:B:166:LEU:HA	1.82	0.42
1:B:192:THR:HG23	1:B:193:ALA:N	2.34	0.42
1:A:121:PRO:HD2	1:A:122:THR:H	1.84	0.42
1:A:265:LYS:HZ3	1:A:271:ALA:HB3	1.84	0.42
1:A:228:PHE:HB2	1:A:235:ALA:HB2	2.02	0.42
1:B:178:GLN:CG	1:B:243:ALA:HB2	2.49	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:309:GLN:NE2	1:B:309:GLN:CA	2.67	0.42
1:B:34:SER:O	1:B:38:THR:HG23	2.20	0.41
1:B:41:VAL:CG2	1:B:43:GLU:CG	2.95	0.41
1:A:63:ARG:HB2	1:A:89:ILE:HG21	2.01	0.41
1:B:38:THR:C	1:B:40:ALA:H	2.27	0.41
1:A:53:ILE:HA	1:A:54:PRO:HD3	1.88	0.41
1:B:33:GLN:O	1:B:37:LEU:HG	2.19	0.41
1:B:121:PRO:O	1:B:125:GLU:N	2.51	0.41
1:A:84:PHE:CE1	1:A:155:ALA:HB1	2.55	0.41
1:A:162:VAL:CG2	1:A:232:PRO:HG3	2.50	0.41
1:B:48:THR:HA	1:B:64:VAL:O	2.19	0.41
1:A:38:THR:HG22	1:A:94:HIS:ND1	2.36	0.41
1:A:286:PHE:C	1:A:288:PRO:HD2	2.45	0.41
1:B:162:VAL:HG21	1:B:229:LYS:O	2.21	0.41
1:B:168:ARG:NH1	1:B:238:GLY:O	2.50	0.41
1:B:223:GLU:C	1:B:225:ALA:N	2.77	0.41
1:B:285:SER:HB2	2:B:2024:HOH:O	2.21	0.41
1:B:309:GLN:HE21	1:B:309:GLN:CA	2.33	0.41
1:A:144:ASP:HA	1:A:145:PRO:HD2	1.84	0.40
1:B:192:THR:CG2	1:B:193:ALA:N	2.84	0.40
1:B:61:ARG:HG2	1:B:89:ILE:HD12	2.03	0.40
1:B:63:ARG:HG2	1:B:65:TYR:CE2	2.56	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:A:26:LEU:HD12	1:A:26:LEU:HA	1.81	0.40
1:B:192:THR:HG22	1:B:194:SER:N	2.36	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	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ASP:N	1:B:221:ARG:NH2[6_455]	1.63	0.57

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

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 [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	233/244 (96%)	207 (89%)	26 (11%)	6	7
1	B	230/244 (94%)	193 (84%)	37 (16%)	2	2
All	All	463/488 (95%)	400 (86%)	63 (14%)	3	4

All (63) 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	91	THR
1	A	94	HIS
1	A	108	VAL
1	A	173	LYS
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	294	ARG
1	A	297	LEU
1	A	304	ILE
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

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Mol	Chain	Res	Type
1	B	99	LEU
1	B	104	ASP
1	B	108	VAL
1	B	111	ASP
1	B	121	PRO
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	209	GLU
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
1	B	290	VAL

Sometimes 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 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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	115:ALA	C	116:PRO	N	1.75
1	B	98:ARG	C	99:LEU	N	1.11
1	B	203:THR	C	204:THR	N	1.06

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	291/311 (93%)	1.86	103 (35%) 1 1	6, 16, 31, 42	3 (1%)
1	B	287/311 (92%)	1.10	36 (12%) 8 9	0, 0, 0, 0	0
All	All	578/622 (92%)	1.48	139 (24%) 2 2	0, 7, 28, 42	3 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	SER	10.7
1	A	33	GLN	6.8
1	A	17	LEU	6.1
1	A	202	GLU	6.1
1	A	220	LYS	5.9
1	A	221	ARG	5.8
1	A	203	THR	5.4
1	B	221	ARG	5.2
1	A	173	LYS	5.0
1	A	56	SER	4.8
1	A	41	VAL	4.7
1	B	41	VAL	4.7
1	A	286	PHE	4.6
1	A	68	LYS	4.5
1	B	202	GLU	4.4
1	A	50	ASP	4.3
1	B	121	PRO	4.3
1	B	33	GLN	4.3
1	A	139	ASP	4.2
1	A	205	SER	4.2
1	B	310	PRO	4.1
1	A	48	THR	4.0
1	A	69	LYS	4.0
1	A	141	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	61	ARG	4.0
1	B	189	GLY	3.9
1	B	25	GLU	3.9
1	B	26	LEU	3.9
1	A	71	ALA	3.9
1	A	36	LEU	3.9
1	B	21	ALA	3.9
1	A	35	ARG	3.8
1	A	270	ARG	3.8
1	A	18	SER	3.7
1	B	86	PHE	3.7
1	A	46	ALA	3.6
1	A	294	ARG	3.6
1	B	203	THR	3.6
1	B	140	GLU	3.5
1	A	265	LYS	3.4
1	A	49	ARG	3.4
1	A	310	PRO	3.3
1	A	28	ARG	3.3
1	A	101	ARG	3.3
1	B	22	SER	3.3
1	A	120	PHE	3.3
1	A	191	PRO	3.1
1	B	37	LEU	3.1
1	B	204	THR	3.1
1	B	136	ASP	3.1
1	A	58	GLY	3.0
1	A	200	VAL	3.0
1	A	226	TYR	3.0
1	A	140	GLU	3.0
1	A	44	PRO	3.0
1	A	32	GLU	2.9
1	A	19	ILE	2.9
1	A	99	LEU	2.9
1	A	87	GLY	2.8
1	A	121	PRO	2.8
1	A	288	PRO	2.8
1	A	298	ASP	2.8
1	A	97	ARG	2.8
1	B	42	GLN	2.8
1	A	143	VAL	2.8
1	A	52	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	2.8
1	B	40	ALA	2.7
1	B	274	VAL	2.7
1	A	146	ASP	2.7
1	A	108	VAL	2.7
1	A	47	GLU	2.7
1	A	287	TYR	2.7
1	B	289	PHE	2.7
1	A	204	THR	2.7
1	B	139	ASP	2.7
1	A	39	ALA	2.6
1	A	67	PRO	2.6
1	A	142	GLY	2.6
1	A	289	PHE	2.6
1	A	51	VAL	2.6
1	B	122	THR	2.5
1	A	76	VAL	2.5
1	A	57	GLY	2.5
1	A	222	PRO	2.5
1	B	222	PRO	2.5
1	B	286	PHE	2.5
1	A	280	VAL	2.5
1	A	118	TYR	2.5
1	B	137	ARG	2.5
1	B	216	ARG	2.5
1	A	128	TYR	2.5
1	A	34	SER	2.4
1	A	59	SER	2.4
1	A	66	PHE	2.4
1	A	213	TRP	2.4
1	A	259	LEU	2.4
1	A	138	ALA	2.4
1	A	239	GLY	2.4
1	B	294	ARG	2.4
1	A	70	ALA	2.4
1	A	137	ARG	2.4
1	A	104	ASP	2.4
1	B	35	ARG	2.4
1	A	38	THR	2.3
1	A	89	ILE	2.3
1	B	223	GLU	2.3
1	A	42	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	214	PHE	2.3
1	A	136	ASP	2.3
1	A	60	ILE	2.3
1	B	68	LYS	2.3
1	A	86	PHE	2.2
1	B	55	VAL	2.3
1	A	63	ARG	2.2
1	A	122	THR	2.2
1	A	37	LEU	2.2
1	A	174	LEU	2.2
1	A	54	PRO	2.2
1	A	72	GLY	2.2
1	B	87	GLY	2.2
1	A	216	ARG	2.2
1	B	97	ARG	2.2
1	A	235	ALA	2.2
1	A	45	ILE	2.1
1	A	212	VAL	2.1
1	B	38	THR	2.1
1	A	55	VAL	2.1
1	A	106	VAL	2.1
1	A	40	ALA	2.1
1	A	161	ALA	2.1
1	A	85	VAL	2.1
1	A	188	THR	2.1
1	A	206	LEU	2.1
1	A	163	VAL	2.1
1	A	201	ALA	2.0
1	B	90	GLU	2.0
1	A	246	VAL	2.0
1	A	290	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.