



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:18 PM UTC

PDB ID : 1KEZ / pdb_00001kez
Title : Crystal Structure of the Macrocycle-forming Thioesterase Domain of Erythromycin Polyketide Synthase (DEBS TE)
Authors : Tsai, S.-C.; Miercke, L.J.W.; Krucinski, J.; Gokhale, R.; Chen, J.C.-H.; Foster, P.G.; Cane, D.E.; Khosla, C.; Stroud, R.M.
Deposited on : 2001-11-19
Resolution : 2.80 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
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

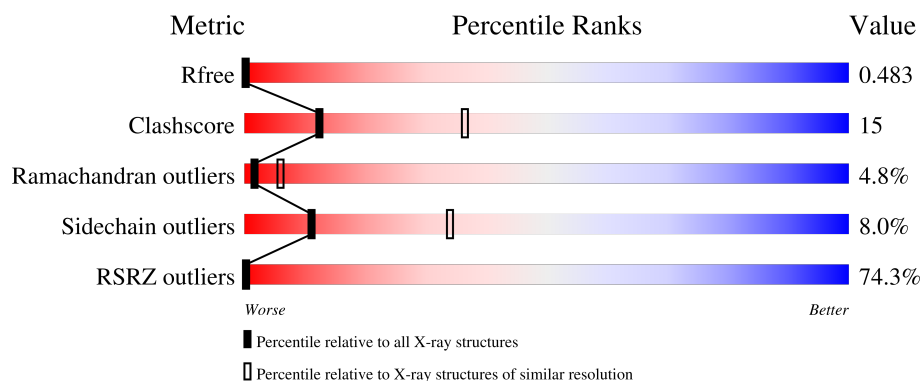
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	300	67% 60% 24% 5% 11%
1	B	300	57% 56% 25% 8% 11%
1	C	300	74% 58% 28% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6426 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 ERYTHRONOLIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total 2011	C 1263	N 355	O 384	S 9	0	0	0
1	B	267	Total 2011	C 1263	N 355	O 384	S 9	0	0	0
1	C	267	Total 2011	C 1263	N 355	O 384	S 9	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q03133
A	2	ALA	-	cloning artifact	UNP Q03133
A	3	SER	-	cloning artifact	UNP Q03133
A	284	SER	-	expression tag	UNP Q03133
A	285	SER	-	expression tag	UNP Q03133
A	286	VAL	-	expression tag	UNP Q03133
A	287	ASP	-	expression tag	UNP Q03133
A	288	LYS	-	expression tag	UNP Q03133
A	289	LEU	-	expression tag	UNP Q03133
A	290	ALA	-	expression tag	UNP Q03133
A	291	ALA	-	expression tag	UNP Q03133
A	292	ALA	-	expression tag	UNP Q03133
A	293	LEU	-	expression tag	UNP Q03133
A	294	GLU	-	expression tag	UNP Q03133
A	295	HIS	-	expression tag	UNP Q03133
A	296	HIS	-	expression tag	UNP Q03133
A	297	HIS	-	expression tag	UNP Q03133
A	298	HIS	-	expression tag	UNP Q03133
A	299	HIS	-	expression tag	UNP Q03133
A	300	HIS	-	expression tag	UNP Q03133
B	1	MET	-	cloning artifact	UNP Q03133
B	2	ALA	-	cloning artifact	UNP Q03133
B	3	SER	-	cloning artifact	UNP Q03133

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Chain	Residue	Modelled	Actual	Comment	Reference
B	284	SER	-	expression tag	UNP Q03133
B	285	SER	-	expression tag	UNP Q03133
B	286	VAL	-	expression tag	UNP Q03133
B	287	ASP	-	expression tag	UNP Q03133
B	288	LYS	-	expression tag	UNP Q03133
B	289	LEU	-	expression tag	UNP Q03133
B	290	ALA	-	expression tag	UNP Q03133
B	291	ALA	-	expression tag	UNP Q03133
B	292	ALA	-	expression tag	UNP Q03133
B	293	LEU	-	expression tag	UNP Q03133
B	294	GLU	-	expression tag	UNP Q03133
B	295	HIS	-	expression tag	UNP Q03133
B	296	HIS	-	expression tag	UNP Q03133
B	297	HIS	-	expression tag	UNP Q03133
B	298	HIS	-	expression tag	UNP Q03133
B	299	HIS	-	expression tag	UNP Q03133
B	300	HIS	-	expression tag	UNP Q03133
C	1	MET	-	cloning artifact	UNP Q03133
C	2	ALA	-	cloning artifact	UNP Q03133
C	3	SER	-	cloning artifact	UNP Q03133
C	284	SER	-	expression tag	UNP Q03133
C	285	SER	-	expression tag	UNP Q03133
C	286	VAL	-	expression tag	UNP Q03133
C	287	ASP	-	expression tag	UNP Q03133
C	288	LYS	-	expression tag	UNP Q03133
C	289	LEU	-	expression tag	UNP Q03133
C	290	ALA	-	expression tag	UNP Q03133
C	291	ALA	-	expression tag	UNP Q03133
C	292	ALA	-	expression tag	UNP Q03133
C	293	LEU	-	expression tag	UNP Q03133
C	294	GLU	-	expression tag	UNP Q03133
C	295	HIS	-	expression tag	UNP Q03133
C	296	HIS	-	expression tag	UNP Q03133
C	297	HIS	-	expression tag	UNP Q03133
C	298	HIS	-	expression tag	UNP Q03133
C	299	HIS	-	expression tag	UNP Q03133
C	300	HIS	-	expression tag	UNP Q03133

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	83	Total O 83 83	0	0

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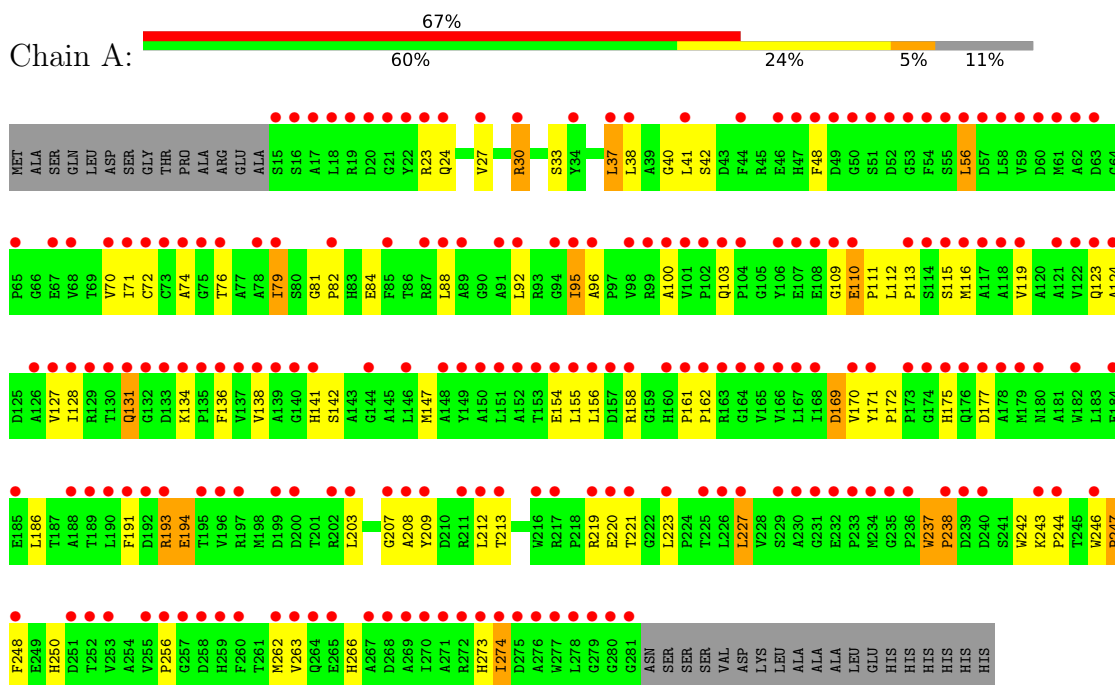
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	217	Total	O	0	0
			217	217		
2	C	93	Total	O	0	0
			93	93		

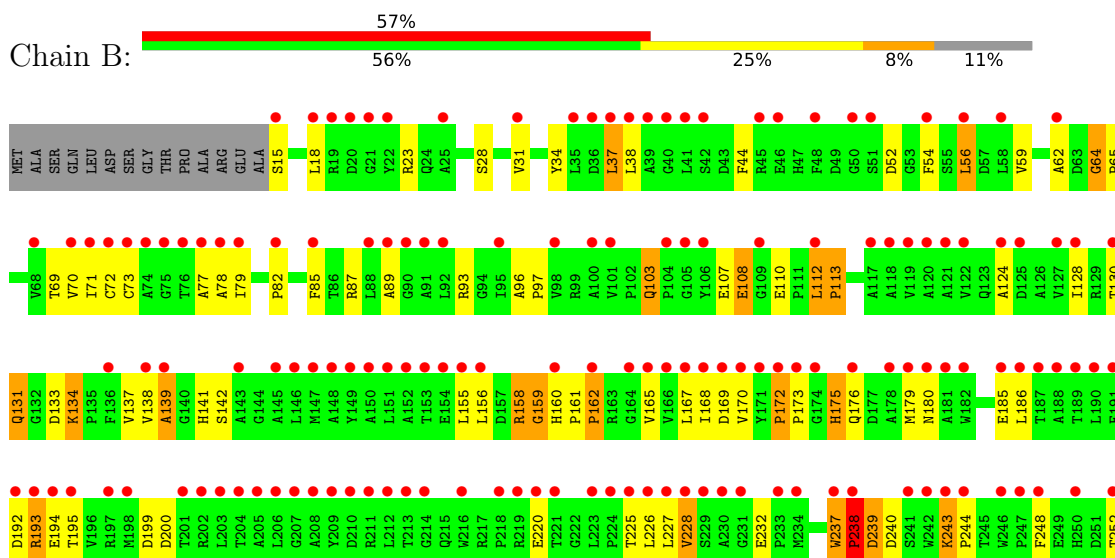
3 Residue-property plots

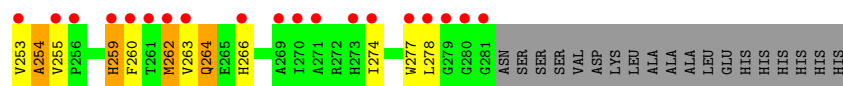
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ERYTHRONOLIDE SYNTHASE

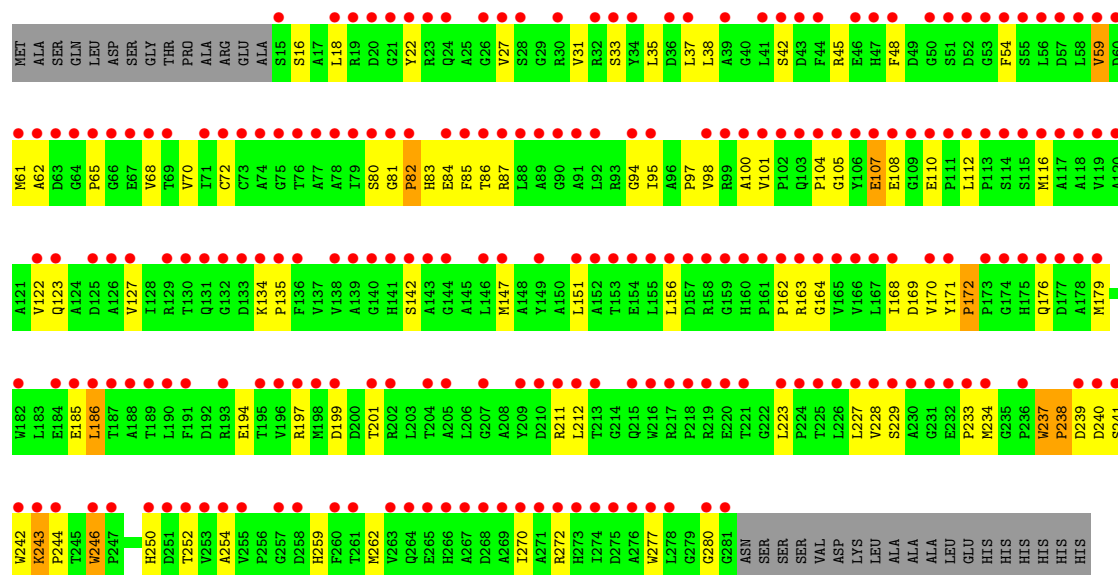
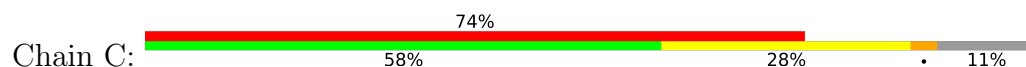


• Molecule 1: ERYTHRONOLIDE SYNTHASE





● Molecule 1: ERYTHRONOLIDE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.50Å 130.50Å 208.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.80) 89.7 (30.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.81Å)	Xtriage
Refinement program	CNS, XTALVIEW	Depositor
R, R_{free}	0.254 , 0.279 0.475 , 0.483	Depositor DCC
R_{free} test set	2278 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	6426	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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	0.46	0/2065	0.94	8/2821 (0.3%)
1	B	0.55	0/2065	1.12	19/2821 (0.7%)
1	C	0.47	0/2065	0.99	12/2821 (0.4%)
All	All	0.50	0/6195	1.02	39/8463 (0.5%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	GLY	CA-C-N	8.14	129.22	120.11
1	B	64	GLY	C-N-CA	8.14	129.22	120.11
1	B	237	TRP	CA-C-N	7.43	129.13	119.84
1	B	237	TRP	C-N-CA	7.43	129.13	119.84
1	B	44	PHE	N-CA-C	7.16	119.80	109.71
1	C	27	VAL	N-CA-C	7.15	117.91	110.62
1	C	254	ALA	N-CA-C	6.91	119.65	110.53
1	C	171	TYR	CA-C-N	6.76	127.34	120.38
1	C	171	TYR	C-N-CA	6.76	127.34	120.38
1	B	252	THR	N-CA-C	6.67	119.87	109.52
1	B	161	PRO	CA-C-N	6.58	128.07	119.84
1	B	161	PRO	C-N-CA	6.58	128.07	119.84
1	B	193	ARG	N-CA-C	6.36	118.50	110.24
1	B	254	ALA	N-CA-C	6.34	119.68	109.79
1	B	179	MET	N-CA-C	6.32	118.69	111.11
1	A	110	GLU	N-CA-C	6.27	117.55	109.65
1	B	232	GLU	CA-C-N	6.13	126.09	119.78
1	B	232	GLU	C-N-CA	6.13	126.09	119.78
1	A	246	TRP	CA-C-N	6.11	127.47	119.84
1	A	246	TRP	C-N-CA	6.11	127.47	119.84
1	B	172	PRO	CA-C-N	6.03	126.86	120.11
1	B	172	PRO	C-N-CA	6.03	126.86	120.11
1	B	156	LEU	N-CA-C	5.65	117.11	111.07
1	C	237	TRP	CA-C-N	5.56	126.79	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	TRP	C-N-CA	5.56	126.79	119.84
1	C	172	PRO	CA-C-N	5.55	125.50	119.78
1	C	172	PRO	C-N-CA	5.55	125.50	119.78
1	C	246	TRP	CA-C-N	5.54	125.06	119.19
1	C	246	TRP	C-N-CA	5.54	125.06	119.19
1	C	59	VAL	N-CA-C	5.45	116.57	108.23
1	C	201	THR	N-CA-C	5.42	117.19	111.28
1	B	112	LEU	CA-C-N	5.36	126.54	119.84
1	B	112	LEU	C-N-CA	5.36	126.54	119.84
1	A	109	GLY	N-CA-C	5.17	120.96	114.25
1	A	172	PRO	CA-C-N	5.07	125.05	120.03
1	A	172	PRO	C-N-CA	5.07	125.05	120.03
1	A	171	TYR	CA-C-N	5.06	125.60	120.38
1	A	171	TYR	C-N-CA	5.06	125.60	120.38
1	B	110	GLU	N-CA-C	5.00	117.73	109.58

There are no chirality outliers.

There are no planarity outliers.

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	2011	0	1925	65	0
1	B	2011	0	1925	69	0
1	C	2011	0	1925	52	0
2	A	83	0	0	12	0
2	B	217	0	0	25	0
2	C	93	0	0	2	0
All	All	6426	0	5775	182	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 15.

All (182) 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:69:THR:HG23	1:B:97:PRO:HB2	1.53	0.90
1:C:107:GLU:HG3	1:C:108:GLU:N	1.98	0.78
1:A:71:ILE:HD13	1:A:136:PHE:HB2	1.67	0.76
1:A:169:ASP:HA	1:A:244:PRO:HG3	1.69	0.74
1:A:194:GLU:H	1:A:194:GLU:CD	1.95	0.74
1:C:186:LEU:HG	1:C:234:MET:HE3	1.69	0.74
1:A:74:ALA:HB3	1:A:103:GLN:HG2	1.70	0.73
1:B:131:GLN:NE2	1:B:134:LYS:HB3	2.03	0.73
1:A:115:SER:HA	1:A:212:LEU:HD22	1.69	0.72
1:B:73:CYS:HB2	2:B:463:HOH:O	1.88	0.72
1:A:79:ILE:H	1:A:79:ILE:HD13	1.56	0.71
1:B:228:VAL:HA	1:B:253:VAL:O	1.91	0.69
1:A:37:LEU:HD12	1:B:37:LEU:HD22	1.75	0.68
1:A:48:PHE:HD2	1:A:111:PRO:HB2	1.59	0.67
1:B:103:GLN:HE21	1:B:103:GLN:HA	1.58	0.67
1:A:208:ALA:O	1:A:212:LEU:HG	1.94	0.67
1:C:105:GLY:HA2	1:C:110:GLU:O	1.97	0.65
1:C:107:GLU:HG3	1:C:108:GLU:H	1.60	0.65
1:B:158:ARG:HD3	2:B:303:HOH:O	1.98	0.64
1:B:262:MET:HG3	1:B:263:VAL:H	1.62	0.64
1:B:54:PHE:HE1	2:B:517:HOH:O	1.80	0.63
1:A:56:LEU:HD11	1:A:123:GLN:HG2	1.81	0.63
1:B:165:VAL:HB	2:B:321:HOH:O	1.98	0.62
1:C:82:PRO:HB3	1:C:100:ALA:HB1	1.80	0.62
1:A:37:LEU:O	1:B:37:LEU:HD11	2.00	0.61
1:A:38:LEU:HB2	1:A:207:GLY:HA3	1.82	0.61
1:C:116:MET:SD	1:C:212:LEU:HB3	2.41	0.61
1:B:62:ALA:HB2	2:B:472:HOH:O	2.02	0.60
1:C:72:CYS:O	1:C:100:ALA:HA	2.03	0.59
1:C:237:TRP:HE1	1:C:241:SER:HB3	1.68	0.58
1:C:142:SER:HA	1:C:170:VAL:HA	1.85	0.58
1:A:92:LEU:HB3	1:A:96:ALA:O	2.03	0.58
1:A:116:MET:HE1	1:A:147:MET:SD	2.44	0.58
1:A:128:ILE:HD12	1:A:158:ARG:HH21	1.66	0.58
1:A:162:PRO:O	1:A:223:LEU:HD22	2.03	0.58
1:A:95:ILE:H	1:A:95:ILE:HD12	1.69	0.57
1:A:113:PRO:HD3	2:A:379:HOH:O	2.04	0.57
1:A:88:LEU:HD22	2:A:323:HOH:O	2.05	0.56
1:B:170:VAL:HG22	2:B:373:HOH:O	2.05	0.56
1:A:142:SER:HA	1:A:170:VAL:HA	1.88	0.56
1:C:59:VAL:HB	1:C:100:ALA:HB3	1.87	0.56
1:A:242:TRP:O	1:A:243:LYS:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD23	1:B:34:TYR:HE1	1.71	0.56
1:B:89:ALA:O	1:B:93:ARG:HG3	2.06	0.55
1:A:119:VAL:HG11	1:A:147:MET:HE1	1.87	0.55
1:A:48:PHE:CD2	1:A:111:PRO:HB2	2.41	0.55
1:C:162:PRO:HG2	1:C:223:LEU:HD13	1.89	0.54
1:B:69:THR:CG2	1:B:97:PRO:HB2	2.32	0.54
1:A:33:SER:O	1:A:37:LEU:HD22	2.08	0.54
1:C:105:GLY:HA3	1:C:112:LEU:HD23	1.90	0.54
1:C:116:MET:HE1	1:C:147:MET:SD	2.48	0.53
1:A:273:HIS:HB3	2:A:377:HOH:O	2.09	0.53
1:A:76:THR:HG22	1:A:76:THR:O	2.09	0.52
1:B:96:ALA:HB3	2:B:350:HOH:O	2.09	0.52
1:B:162:PRO:HB3	2:B:442:HOH:O	2.09	0.52
1:C:164:GLY:HA3	1:C:277:TRP:CH2	2.45	0.52
1:A:24:GLN:O	1:A:27:VAL:HG22	2.10	0.52
1:C:179:MET:SD	1:C:237:TRP:CZ2	3.03	0.52
1:C:227:LEU:HD23	1:C:228:VAL:O	2.10	0.52
1:B:274:ILE:HG21	2:B:335:HOH:O	2.09	0.52
1:A:24:GLN:NE2	1:A:27:VAL:HG21	2.25	0.51
1:B:70:VAL:HG22	1:B:137:VAL:CG2	2.40	0.51
1:B:103:GLN:HB3	2:B:358:HOH:O	2.10	0.51
1:B:141:HIS:HE1	1:B:262:MET:SD	2.33	0.51
1:A:266:HIS:HA	2:A:309:HOH:O	2.09	0.51
1:A:227:LEU:HB2	1:A:250:HIS:HD2	1.74	0.51
1:A:42:SER:HB2	1:A:112:LEU:HD13	1.93	0.51
1:A:95:ILE:HD12	1:A:95:ILE:N	2.25	0.51
1:A:131:GLN:HE21	1:A:134:LYS:HB3	1.74	0.51
1:A:175:HIS:CE1	2:A:319:HOH:O	2.63	0.51
1:C:35:LEU:HD23	1:C:38:LEU:HD12	1.92	0.51
1:C:169:ASP:HA	1:C:244:PRO:HG3	1.92	0.51
1:A:123:GLN:O	1:A:127:VAL:HG23	2.11	0.51
1:C:33:SER:O	1:C:37:LEU:HD23	2.11	0.51
1:C:68:VAL:HG22	1:C:135:PRO:HB2	1.93	0.51
1:B:131:GLN:OE1	1:B:131:GLN:HA	2.12	0.50
1:B:82:PRO:HB3	2:B:407:HOH:O	2.11	0.50
1:A:274:ILE:HG21	2:A:304:HOH:O	2.12	0.50
1:B:220:GLU:HG2	1:B:248:PHE:CE1	2.47	0.50
1:B:255:VAL:HG12	2:B:404:HOH:O	2.11	0.49
1:A:209:TYR:CD2	1:A:212:LEU:HD12	2.47	0.49
1:A:42:SER:HB2	1:A:112:LEU:CD1	2.42	0.49
1:B:167:LEU:HB2	1:B:227:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LEU:O	1:C:22:TYR:HB2	2.12	0.49
1:C:135:PRO:HB3	1:C:163:ARG:HE	1.78	0.49
1:A:250:HIS:HB3	2:A:341:HOH:O	2.13	0.48
1:B:141:HIS:CG	1:B:142:SER:N	2.80	0.48
1:A:72:CYS:O	1:A:100:ALA:HA	2.13	0.48
1:B:71:ILE:HG22	1:B:72:CYS:N	2.28	0.48
1:B:124:ALA:O	1:B:128:ILE:HG13	2.13	0.48
1:A:30:ARG:HB2	2:A:360:HOH:O	2.12	0.48
1:B:262:MET:O	1:B:266:HIS:HB2	2.14	0.48
1:A:124:ALA:HB1	1:A:155:LEU:HD21	1.96	0.48
1:B:141:HIS:CE1	1:B:262:MET:SD	3.07	0.48
1:B:172:PRO:HA	1:B:173:PRO:HD3	1.76	0.48
1:A:115:SER:CA	1:A:212:LEU:HD22	2.40	0.47
1:B:15:SER:HA	2:B:475:HOH:O	2.14	0.47
1:B:264:GLN:HG2	2:B:312:HOH:O	2.14	0.47
1:A:40:GLY:HA3	1:B:37:LEU:HD21	1.95	0.47
1:C:80:SER:O	1:C:83:HIS:NE2	2.48	0.47
1:C:123:GLN:O	1:C:127:VAL:HG23	2.15	0.47
1:A:112:LEU:HA	2:A:379:HOH:O	2.14	0.47
1:C:31:VAL:HG21	1:C:185:GLU:HA	1.97	0.47
1:A:71:ILE:O	1:A:138:VAL:HA	2.15	0.47
1:A:113:PRO:HG2	1:A:119:VAL:HB	1.97	0.47
1:B:65:PRO:O	1:B:96:ALA:HA	2.15	0.47
1:B:262:MET:HE2	1:B:263:VAL:HG23	1.96	0.47
1:B:69:THR:HB	2:B:436:HOH:O	2.15	0.46
1:C:246:TRP:HB3	1:C:250:HIS:CE1	2.51	0.46
1:A:70:VAL:HG12	1:A:72:CYS:SG	2.56	0.46
1:B:254:ALA:O	1:B:255:VAL:HG23	2.16	0.46
1:B:138:VAL:HG12	1:B:139:ALA:H	1.80	0.46
1:C:70:VAL:HG12	1:C:72:CYS:SG	2.55	0.46
1:C:229:SER:OG	1:C:243:LYS:HG3	2.16	0.46
1:B:69:THR:HG22	1:B:70:VAL:N	2.31	0.45
1:B:128:ILE:O	1:B:128:ILE:HG22	2.15	0.45
1:C:84:GLU:C	1:C:86:THR:H	2.24	0.45
1:C:81:GLY:O	1:C:84:GLU:HG2	2.15	0.45
1:C:164:GLY:HA3	1:C:277:TRP:HH2	1.81	0.45
1:C:170:VAL:O	1:C:172:PRO:HD3	2.16	0.45
1:B:64:GLY:O	1:B:97:PRO:HG3	2.16	0.45
1:B:173:PRO:HG2	2:B:370:HOH:O	2.15	0.45
1:C:101:VAL:HG11	1:C:123:GLN:HB3	1.97	0.45
1:A:48:PHE:CE1	1:A:113:PRO:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:CYS:SG	1:C:98:VAL:HG13	2.56	0.45
1:C:105:GLY:HA3	1:C:112:LEU:CD2	2.46	0.45
1:A:194:GLU:CD	1:A:194:GLU:N	2.71	0.45
1:C:168:ILE:HD13	1:C:270:ILE:HD13	1.98	0.45
1:A:48:PHE:HE2	1:A:111:PRO:O	2.00	0.45
1:C:59:VAL:HG12	1:C:61:MET:SD	2.57	0.45
1:A:203:LEU:HD23	2:A:380:HOH:O	2.17	0.44
1:B:112:LEU:HG	2:B:473:HOH:O	2.16	0.44
1:B:38:LEU:HB3	2:B:378:HOH:O	2.17	0.44
1:B:23:ARG:HB2	2:B:484:HOH:O	2.17	0.44
1:C:59:VAL:HG21	1:C:82:PRO:HB2	2.00	0.44
1:A:220:GLU:HG2	1:A:221:THR:N	2.33	0.43
1:C:233:PRO:HG3	1:C:242:TRP:CH2	2.53	0.43
1:C:65:PRO:O	1:C:97:PRO:HD3	2.18	0.43
1:A:247:PRO:HG2	1:A:248:PHE:H	1.83	0.43
1:B:239:ASP:HB2	1:B:240:ASP:H	1.64	0.43
1:A:116:MET:SD	1:A:213:THR:HG22	2.59	0.43
1:B:31:VAL:HA	2:B:330:HOH:O	2.18	0.43
1:C:48:PHE:HE1	1:C:122:VAL:HG21	1.83	0.43
1:C:62:ALA:HB3	2:C:332:HOH:O	2.19	0.43
1:B:226:LEU:HD22	1:B:277:TRP:CG	2.53	0.43
1:C:233:PRO:HG3	1:C:242:TRP:CZ2	2.54	0.43
1:B:18:LEU:HD22	2:B:401:HOH:O	2.19	0.42
1:A:33:SER:HB2	2:A:360:HOH:O	2.19	0.42
1:A:110:GLU:HA	1:A:111:PRO:HD3	1.75	0.42
1:B:87:ARG:NH1	1:B:264:GLN:NE2	2.67	0.42
1:B:113:PRO:HD2	2:B:316:HOH:O	2.19	0.42
1:B:124:ALA:HB1	2:B:303:HOH:O	2.20	0.42
1:C:151:LEU:HD22	2:C:312:HOH:O	2.18	0.42
1:C:54:PHE:HE1	1:C:104:PRO:HB2	1.84	0.42
1:C:172:PRO:HD2	1:C:176:GLN:OE1	2.20	0.42
1:C:134:LYS:HA	1:C:135:PRO:HD3	1.87	0.42
1:B:56:LEU:HD12	2:B:318:HOH:O	2.20	0.42
1:A:127:VAL:O	1:A:131:GLN:HB2	2.19	0.42
1:A:262:MET:HG3	1:A:263:VAL:HG23	2.01	0.42
1:B:259:HIS:ND1	1:B:259:HIS:C	2.78	0.42
1:B:237:TRP:HA	1:B:238:PRO:HD3	1.85	0.42
1:B:85:PHE:C	1:B:87:ARG:H	2.26	0.41
1:B:138:VAL:HG12	1:B:139:ALA:N	2.35	0.41
1:C:259:HIS:O	1:C:262:MET:HG2	2.20	0.41
1:A:81:GLY:O	1:A:84:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ILE:HG22	1:B:72:CYS:H	1.83	0.41
1:C:168:ILE:HG12	1:C:228:VAL:HG21	2.00	0.41
1:A:161:PRO:HA	1:A:162:PRO:HD2	1.96	0.41
1:B:71:ILE:O	1:B:72:CYS:SG	2.73	0.41
1:B:278:LEU:HA	2:B:380:HOH:O	2.20	0.41
1:B:31:VAL:HG21	1:B:185:GLU:HA	2.01	0.41
1:A:156:LEU:HD22	1:A:221:THR:OG1	2.21	0.41
1:B:64:GLY:HA2	1:B:65:PRO:HD3	1.80	0.41
1:C:237:TRP:HA	1:C:238:PRO:HD3	1.78	0.41
1:C:238:PRO:HB2	1:C:239:ASP:H	1.61	0.41
1:A:237:TRP:HA	1:A:238:PRO:HD3	1.84	0.40
1:B:56:LEU:HD23	1:B:56:LEU:N	2.36	0.40
1:B:85:PHE:C	1:B:87:ARG:N	2.79	0.40
1:C:42:SER:O	1:C:45:ARG:HB2	2.20	0.40
1:B:159:GLY:O	1:B:160:HIS:CG	2.75	0.40
1:B:243:LYS:HA	1:B:244:PRO:HD3	1.87	0.40
1:A:141:HIS:HB3	2:A:303:HOH:O	2.22	0.40

There are no symmetry-related clashes.

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	265/300 (88%)	219 (83%)	39 (15%)	7 (3%)	4	15
1	B	265/300 (88%)	189 (71%)	54 (20%)	22 (8%)	0	1
1	C	265/300 (88%)	218 (82%)	38 (14%)	9 (3%)	3	11
All	All	795/900 (88%)	626 (79%)	131 (16%)	38 (5%)	2	6

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ARG
1	A	238	PRO
1	B	78	ALA
1	B	131	GLN
1	B	200	ASP
1	B	238	PRO
1	B	259	HIS
1	B	264	GLN
1	C	238	PRO
1	A	131	GLN
1	B	107	GLU
1	B	133	ASP
1	B	180	ASN
1	B	262	MET
1	C	85	PHE
1	C	156	LEU
1	C	240	ASP
1	C	280	GLY
1	A	256	PRO
1	B	77	ALA
1	B	162	PRO
1	B	169	ASP
1	B	243	LYS
1	B	260	PHE
1	C	243	LYS
1	B	79	ILE
1	B	175	HIS
1	B	52	ASP
1	C	95	ILE
1	A	247	PRO
1	B	108	GLU
1	B	113	PRO
1	B	139	ALA
1	A	95	ILE
1	B	159	GLY
1	A	82	PRO
1	C	82	PRO
1	C	94	GLY

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	204/230 (89%)	188 (92%)	16 (8%)	11	35
1	B	204/230 (89%)	181 (89%)	23 (11%)	5	19
1	C	204/230 (89%)	194 (95%)	10 (5%)	22	55
All	All	612/690 (89%)	563 (92%)	49 (8%)	11	34

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	30	ARG
1	A	37	LEU
1	A	56	LEU
1	A	79	ILE
1	A	154	GLU
1	A	169	ASP
1	A	177	ASP
1	A	186	LEU
1	A	191	PHE
1	A	193	ARG
1	A	194	GLU
1	A	219	ARG
1	A	227	LEU
1	A	237	TRP
1	A	274	ILE
1	B	28	SER
1	B	37	LEU
1	B	56	LEU
1	B	59	VAL
1	B	103	GLN
1	B	108	GLU
1	B	130	THR
1	B	134	LYS
1	B	155	LEU
1	B	158	ARG
1	B	168	ILE
1	B	175	HIS
1	B	176	GLN
1	B	186	LEU

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Mol	Chain	Res	Type
1	B	192	ASP
1	B	193	ARG
1	B	194	GLU
1	B	195	THR
1	B	199	ASP
1	B	225	THR
1	B	228	VAL
1	B	238	PRO
1	B	239	ASP
1	C	16	SER
1	C	87	ARG
1	C	107	GLU
1	C	186	LEU
1	C	194	GLU
1	C	197	ARG
1	C	199	ASP
1	C	211	ARG
1	C	252	THR
1	C	272	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	103	GLN
1	A	123	GLN
1	A	131	GLN
1	A	141	HIS
1	A	250	HIS
1	A	273	HIS
1	B	103	GLN
1	B	141	HIS
1	B	264	GLN
1	C	131	GLN
1	C	250	HIS
1	C	266	HIS

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](#)

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	267/300 (89%)	3.09	202 (75%) 0 0	52, 64, 88, 123	0
1	B	267/300 (89%)	2.94	171 (64%) 0 0	32, 68, 76, 83	0
1	C	267/300 (89%)	3.30	222 (83%) 0 0	52, 64, 90, 118	0
All	All	801/900 (89%)	3.11	595 (74%) 0 0	32, 65, 86, 123	0

All (595) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	ALA	20.4
1	B	167	LEU	14.5
1	A	15	SER	9.8
1	C	229	SER	9.8
1	C	157	ASP	9.5
1	B	227	LEU	9.3
1	C	114	SER	9.3
1	A	157	ASP	9.3
1	B	71	ILE	9.2
1	B	165	VAL	9.0
1	C	189	THR	8.8
1	B	152	ALA	8.8
1	A	108	GLU	8.5
1	C	231	GLY	8.4
1	A	20	ASP	8.3
1	B	166	VAL	8.3
1	B	260	PHE	8.2
1	A	57	ASP	8.2
1	B	168	ILE	8.1
1	C	264	GLN	7.9
1	B	151	LEU	7.8
1	C	281	GLY	7.6
1	A	231	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
1	C	153	THR	7.3
1	C	230	ALA	7.2
1	C	115	SER	6.9
1	B	226	LEU	6.7
1	A	190	LEU	6.6
1	A	74	ALA	6.6
1	A	264	GLN	6.5
1	C	102	PRO	6.5
1	A	212	LEU	6.4
1	C	55	SER	6.4
1	A	277	TRP	6.4
1	C	53	GLY	6.3
1	C	43	ASP	6.3
1	B	56	LEU	6.3
1	B	179	MET	6.3
1	B	92	LEU	6.2
1	A	208	ALA	6.2
1	A	176	GLN	6.2
1	C	185	GLU	6.1
1	A	177	ASP	6.1
1	C	44	PHE	6.1
1	C	188	ALA	6.1
1	B	90	GLY	6.1
1	B	74	ALA	6.1
1	B	88	LEU	6.0
1	C	27	VAL	5.9
1	C	226	LEU	5.9
1	B	40	GLY	5.8
1	C	56	LEU	5.8
1	C	154	GLU	5.7
1	C	57	ASP	5.7
1	A	269	ALA	5.6
1	B	138	VAL	5.6
1	A	192	ASP	5.6
1	A	227	LEU	5.6
1	B	173	PRO	5.6
1	C	108	GLU	5.5
1	C	184	GLU	5.5
1	A	161	PRO	5.5
1	C	123	GLN	5.5
1	A	166	VAL	5.5
1	A	99	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	72	CYS	5.4
1	A	180	ASN	5.4
1	C	76	THR	5.3
1	B	85	PHE	5.3
1	B	58	LEU	5.3
1	B	73	CYS	5.2
1	B	174	GLY	5.2
1	C	198	MET	5.2
1	A	154	GLU	5.2
1	C	152	ALA	5.2
1	B	281	GLY	5.2
1	A	209	TYR	5.1
1	B	228	VAL	5.1
1	C	74	ALA	5.1
1	C	228	VAL	5.1
1	A	56	LEU	5.1
1	C	28	SER	5.1
1	A	191	PHE	5.1
1	B	209	TYR	5.1
1	C	118	ALA	5.0
1	A	82	PRO	5.0
1	A	54	PHE	5.0
1	C	215	GLN	5.0
1	B	118	ALA	5.0
1	C	78	ALA	5.0
1	A	98	VAL	5.0
1	C	178	ALA	5.0
1	A	52	ASP	5.0
1	A	115	SER	4.9
1	B	89	ALA	4.9
1	B	221	THR	4.9
1	A	232	GLU	4.9
1	B	127	VAL	4.9
1	A	22	TYR	4.9
1	A	104	PRO	4.9
1	A	58	LEU	4.9
1	C	133	ASP	4.9
1	A	140	GLY	4.9
1	A	178	ALA	4.9
1	A	213	THR	4.9
1	B	201	THR	4.8
1	A	114	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	72	CYS	4.8
1	A	122	VAL	4.8
1	B	149	TYR	4.8
1	C	103	GLN	4.8
1	C	134	LYS	4.8
1	C	211	ARG	4.8
1	A	171	TYR	4.8
1	A	203	LEU	4.8
1	C	270	ILE	4.8
1	B	162	PRO	4.8
1	A	197	ARG	4.7
1	A	73	CYS	4.7
1	B	95	ILE	4.7
1	A	195	THR	4.7
1	C	163	ARG	4.7
1	C	273	HIS	4.7
1	A	220	GLU	4.7
1	B	202	ARG	4.7
1	A	123	GLN	4.6
1	C	82	PRO	4.6
1	C	174	GLY	4.6
1	A	156	LEU	4.5
1	C	156	LEU	4.5
1	B	205	ALA	4.5
1	C	88	LEU	4.5
1	B	156	LEU	4.5
1	B	148	ALA	4.5
1	A	132	GLY	4.5
1	C	219	ARG	4.5
1	B	153	THR	4.5
1	B	218	PRO	4.5
1	C	107	GLU	4.5
1	C	36	ASP	4.4
1	C	261	THR	4.4
1	B	91	ALA	4.4
1	C	277	TRP	4.4
1	C	59	VAL	4.4
1	A	41	LEU	4.4
1	B	37	LEU	4.4
1	C	58	LEU	4.4
1	A	221	THR	4.4
1	C	218	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	166	VAL	4.4
1	C	100	ALA	4.3
1	B	68	VAL	4.3
1	B	120	ALA	4.3
1	C	91	ALA	4.3
1	C	247	PRO	4.3
1	C	146	LEU	4.3
1	A	34	TYR	4.3
1	A	129	ARG	4.3
1	C	272	ARG	4.3
1	C	141	HIS	4.3
1	C	173	PRO	4.3
1	A	62	ALA	4.3
1	B	145	ALA	4.3
1	C	251	ASP	4.3
1	A	71	ILE	4.2
1	C	239	ASP	4.2
1	C	177	ASP	4.2
1	C	84	GLU	4.2
1	B	170	VAL	4.2
1	C	37	LEU	4.2
1	A	50	GLY	4.2
1	C	221	THR	4.2
1	B	277	TRP	4.2
1	A	55	SER	4.2
1	C	227	LEU	4.2
1	A	133	ASP	4.2
1	B	171	TYR	4.1
1	A	61	MET	4.1
1	A	103	GLN	4.1
1	B	82	PRO	4.1
1	A	116	MET	4.1
1	C	225	THR	4.0
1	C	244	PRO	4.0
1	B	243	LYS	4.0
1	C	75	GLY	4.0
1	B	203	LEU	4.0
1	C	41	LEU	4.0
1	A	91	ALA	4.0
1	A	150	ALA	4.0
1	B	100	ALA	4.0
1	C	79	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	167	LEU	4.0
1	A	95	ILE	4.0
1	A	144	GLY	4.0
1	B	191	PHE	4.0
1	C	170	VAL	4.0
1	A	106	TYR	4.0
1	C	127	VAL	4.0
1	A	130	THR	4.0
1	B	79	ILE	3.9
1	A	211	ARG	3.9
1	B	271	ALA	3.9
1	C	276	ALA	3.9
1	A	53	GLY	3.9
1	C	240	ASP	3.9
1	C	232	GLU	3.9
1	B	146	LEU	3.9
1	B	119	VAL	3.9
1	C	98	VAL	3.9
1	A	75	GLY	3.9
1	B	154	GLU	3.9
1	B	128	ILE	3.9
1	A	229	SER	3.9
1	C	209	TYR	3.8
1	C	204	THR	3.8
1	A	88	LEU	3.8
1	C	111	PRO	3.8
1	A	267	ALA	3.8
1	A	223	LEU	3.8
1	C	212	LEU	3.8
1	B	178	ALA	3.8
1	B	48	PHE	3.8
1	C	20	ASP	3.7
1	C	199	ASP	3.7
1	B	216	TRP	3.7
1	C	18	LEU	3.7
1	B	234	MET	3.7
1	B	42	SER	3.7
1	A	270	ILE	3.7
1	B	122	VAL	3.7
1	B	263	VAL	3.7
1	A	256	PRO	3.7
1	B	223	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	66	GLY	3.6
1	C	85	PHE	3.6
1	A	138	VAL	3.6
1	B	274	ILE	3.6
1	A	226	LEU	3.6
1	A	30	ARG	3.6
1	B	256	PRO	3.6
1	B	278	LEU	3.6
1	C	202	ARG	3.6
1	A	274	ILE	3.6
1	A	76	THR	3.6
1	A	273	HIS	3.6
1	C	47	HIS	3.6
1	C	19	ARG	3.6
1	C	33	SER	3.6
1	B	244	PRO	3.6
1	B	143	ALA	3.5
1	A	110	GLU	3.5
1	C	246	TRP	3.5
1	A	68	VAL	3.5
1	B	51	SER	3.5
1	B	185	GLU	3.5
1	C	67	GLU	3.5
1	B	273	HIS	3.5
1	C	175	HIS	3.5
1	A	126	ALA	3.5
1	A	127	VAL	3.5
1	B	98	VAL	3.5
1	A	179	MET	3.5
1	A	162	PRO	3.5
1	C	217	ARG	3.5
1	C	130	THR	3.5
1	B	78	ALA	3.5
1	C	72	CYS	3.5
1	C	46	GLU	3.5
1	A	51	SER	3.5
1	B	246	TRP	3.5
1	C	260	PHE	3.4
1	A	281	GLY	3.4
1	C	138	VAL	3.4
1	B	208	ALA	3.4
1	A	119	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	182	TRP	3.4
1	C	147	MET	3.4
1	A	27	VAL	3.4
1	A	23	ARG	3.4
1	A	244	PRO	3.4
1	B	270	ILE	3.4
1	B	207	GLY	3.4
1	C	165	VAL	3.4
1	A	217	ARG	3.4
1	C	117	ALA	3.4
1	C	54	PHE	3.4
1	B	21	GLY	3.3
1	A	67	GLU	3.3
1	B	220	GLU	3.3
1	A	230	ALA	3.3
1	B	147	MET	3.3
1	C	71	ILE	3.3
1	C	151	LEU	3.3
1	A	174	GLY	3.3
1	B	164	GLY	3.3
1	C	274	ILE	3.3
1	A	149	TYR	3.3
1	C	105	GLY	3.3
1	A	238	PRO	3.3
1	C	158	ARG	3.3
1	C	196	VAL	3.3
1	A	257	GLY	3.3
1	C	51	SER	3.3
1	A	24	GLN	3.3
1	C	210	ASP	3.2
1	B	224	PRO	3.2
1	A	121	ALA	3.2
1	A	109	GLY	3.2
1	B	195	THR	3.2
1	A	16	SER	3.2
1	A	239	ASP	3.2
1	A	117	ALA	3.2
1	B	41	LEU	3.2
1	A	246	TRP	3.2
1	A	236	PRO	3.2
1	C	65	PRO	3.2
1	A	200	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	210	ASP	3.2
1	C	63	ASP	3.2
1	A	18	LEU	3.2
1	B	206	LEU	3.2
1	A	272	ARG	3.2
1	B	38	LEU	3.2
1	C	101	VAL	3.2
1	A	94	GLY	3.2
1	A	278	LEU	3.1
1	C	223	LEU	3.1
1	A	148	ALA	3.1
1	B	39	ALA	3.1
1	A	44	PHE	3.1
1	A	280	GLY	3.1
1	A	89	ALA	3.1
1	B	181	ALA	3.1
1	C	94	GLY	3.1
1	B	186	LEU	3.1
1	B	212	LEU	3.1
1	C	110	GLU	3.1
1	B	213	THR	3.1
1	A	152	ALA	3.1
1	C	60	ASP	3.1
1	B	124	ALA	3.0
1	C	89	ALA	3.0
1	C	191	PHE	3.0
1	A	240	ASP	3.0
1	B	247	PRO	3.0
1	A	165	VAL	3.0
1	C	106	TYR	3.0
1	C	131	GLN	3.0
1	C	139	ALA	3.0
1	A	170	VAL	3.0
1	C	149	TYR	3.0
1	B	197	ARG	3.0
1	C	155	LEU	3.0
1	A	153	THR	3.0
1	B	76	THR	3.0
1	A	260	PHE	3.0
1	B	237	TRP	3.0
1	B	190	LEU	3.0
1	C	90	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	204	THR	3.0
1	B	269	ALA	3.0
1	A	253	VAL	3.0
1	B	255	VAL	3.0
1	C	99	ARG	2.9
1	C	182	TRP	2.9
1	C	242	TRP	2.9
1	B	50	GLY	2.9
1	C	64	GLY	2.9
1	A	118	ALA	2.9
1	A	124	ALA	2.9
1	C	271	ALA	2.9
1	A	160	HIS	2.9
1	C	160	HIS	2.9
1	A	243	LYS	2.9
1	C	73	CYS	2.9
1	C	50	GLY	2.9
1	C	236	PRO	2.9
1	B	242	TRP	2.9
1	A	49	ASP	2.9
1	C	62	ALA	2.9
1	C	143	ALA	2.9
1	C	86	THR	2.9
1	B	233	PRO	2.8
1	A	85	PHE	2.8
1	A	193	ARG	2.8
1	B	261	THR	2.8
1	B	75	GLY	2.8
1	C	234	MET	2.8
1	A	265	GLU	2.8
1	A	188	ALA	2.8
1	A	48	PHE	2.8
1	B	187	THR	2.8
1	B	225	THR	2.8
1	C	140	GLY	2.8
1	C	159	GLY	2.8
1	A	163	ARG	2.8
1	A	219	ARG	2.8
1	A	263	VAL	2.8
1	A	100	ALA	2.8
1	A	155	LEU	2.8
1	B	259	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	180	ASN	2.8
1	C	52	ASP	2.8
1	C	42	SER	2.8
1	A	65	PRO	2.8
1	B	172	PRO	2.8
1	A	141	HIS	2.8
1	A	60	ASP	2.8
1	A	87	ARG	2.7
1	C	220	GLU	2.7
1	A	59	VAL	2.7
1	A	137	VAL	2.7
1	C	205	ALA	2.7
1	B	155	LEU	2.7
1	C	190	LEU	2.7
1	C	69	THR	2.7
1	B	19	ARG	2.7
1	C	265	GLU	2.7
1	A	92	LEU	2.7
1	B	22	TYR	2.7
1	B	241	SER	2.7
1	A	131	GLN	2.7
1	A	136	PHE	2.7
1	C	254	ALA	2.7
1	A	234	MET	2.7
1	B	252	THR	2.7
1	A	102	PRO	2.7
1	B	250	HIS	2.7
1	C	193	ARG	2.7
1	C	197	ARG	2.7
1	C	195	THR	2.7
1	B	36	ASP	2.7
1	C	176	GLN	2.7
1	B	18	LEU	2.7
1	B	35	LEU	2.7
1	B	230	ALA	2.6
1	C	30	ARG	2.6
1	A	207	GLY	2.6
1	C	112	LEU	2.6
1	B	136	PHE	2.6
1	B	262	MET	2.6
1	C	34	TYR	2.6
1	A	173	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	104	PRO	2.6
1	B	130	THR	2.6
1	A	146	LEU	2.6
1	C	278	LEU	2.6
1	A	63	ASP	2.6
1	A	268	ASP	2.6
1	A	17	ALA	2.6
1	B	62	ALA	2.6
1	C	142	SER	2.6
1	A	47	HIS	2.6
1	B	279	GLY	2.6
1	C	104	PRO	2.6
1	A	151	LEU	2.6
1	A	184	GLU	2.6
1	C	168	ILE	2.6
1	B	169	ASP	2.6
1	C	266	HIS	2.6
1	A	202	ARG	2.6
1	B	211	ARG	2.6
1	C	171	TYR	2.6
1	A	252	THR	2.6
1	C	179	MET	2.6
1	B	46	GLU	2.6
1	B	77	ALA	2.6
1	C	23	ARG	2.5
1	C	80	SER	2.5
1	C	135	PRO	2.5
1	C	161	PRO	2.5
1	A	46	GLU	2.5
1	A	96	ALA	2.5
1	C	113	PRO	2.5
1	C	257	GLY	2.5
1	C	213	THR	2.5
1	A	199	ASP	2.5
1	C	125	ASP	2.5
1	B	229	SER	2.5
1	A	70	VAL	2.5
1	A	182	TRP	2.5
1	B	101	VAL	2.5
1	C	77	ALA	2.5
1	C	267	ALA	2.5
1	A	167	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	207	GLY	2.5
1	A	276	ALA	2.5
1	C	126	ALA	2.5
1	B	160	HIS	2.5
1	C	164	GLY	2.4
1	B	125	ASP	2.4
1	B	109	GLY	2.4
1	B	194	GLU	2.4
1	C	22	TYR	2.4
1	B	189	THR	2.4
1	C	201	THR	2.4
1	A	255	VAL	2.4
1	C	109	GLY	2.4
1	C	255	VAL	2.4
1	C	39	ALA	2.4
1	C	224	PRO	2.4
1	C	144	GLY	2.4
1	B	150	ALA	2.4
1	A	175	HIS	2.4
1	C	162	PRO	2.4
1	A	101	VAL	2.3
1	B	248	PHE	2.3
1	C	136	PHE	2.3
1	B	121	ALA	2.3
1	C	61	MET	2.3
1	B	112	LEU	2.3
1	A	271	ALA	2.3
1	B	15	SER	2.3
1	C	15	SER	2.3
1	C	186	LEU	2.3
1	A	259	HIS	2.3
1	A	128	ILE	2.3
1	A	158	ARG	2.3
1	C	233	PRO	2.3
1	B	253	VAL	2.3
1	C	280	GLY	2.3
1	C	48	PHE	2.3
1	A	262	MET	2.3
1	B	176	GLN	2.3
1	A	216	TRP	2.3
1	C	241	SER	2.3
1	A	225	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	214	GLY	2.3
1	A	107	GLU	2.3
1	A	79	ILE	2.3
1	C	250	HIS	2.3
1	B	70	VAL	2.3
1	C	81	GLY	2.3
1	C	120	ALA	2.2
1	C	268	ASP	2.2
1	C	275	ASP	2.2
1	A	139	ALA	2.2
1	C	95	ILE	2.2
1	C	87	ARG	2.2
1	B	106	TYR	2.2
1	B	198	MET	2.2
1	B	45	ARG	2.2
1	C	24	GLN	2.2
1	C	258	ASP	2.2
1	A	134	LYS	2.2
1	C	269	ALA	2.2
1	C	129	ARG	2.2
1	A	251	ASP	2.2
1	C	68	VAL	2.2
1	A	21	GLY	2.2
1	B	105	GLY	2.2
1	A	248	PHE	2.2
1	B	54	PHE	2.2
1	A	37	LEU	2.2
1	A	38	LEU	2.2
1	A	168	ILE	2.1
1	B	31	VAL	2.1
1	A	258	ASP	2.1
1	C	116	MET	2.1
1	A	189	THR	2.1
1	C	92	LEU	2.1
1	A	113	PRO	2.1
1	A	279	GLY	2.1
1	A	19	ARG	2.1
1	C	119	VAL	2.1
1	C	122	VAL	2.1
1	C	263	VAL	2.1
1	B	231	GLY	2.1
1	B	266	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	196	VAL	2.1
1	B	238	PRO	2.1
1	B	280	GLY	2.1
1	B	192	ASP	2.1
1	B	219	ARG	2.1
1	C	32	ARG	2.1
1	A	78	ALA	2.1
1	B	117	ALA	2.1
1	C	216	TRP	2.1
1	A	185	GLU	2.1
1	C	253	VAL	2.0
1	C	132	GLY	2.0
1	A	275	ASP	2.0
1	B	20	ASP	2.0
1	C	243	LYS	2.0
1	A	135	PRO	2.0
1	A	233	PRO	2.0
1	B	193	ARG	2.0
1	A	164	GLY	2.0
1	A	235	GLY	2.0
1	C	21	GLY	2.0
1	C	26	GLY	2.0
1	B	25	ALA	2.0
1	B	188	ALA	2.0
1	C	187	THR	2.0
1	C	252	THR	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.