



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:27 PM GMT

PDB ID : 1KEZ
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

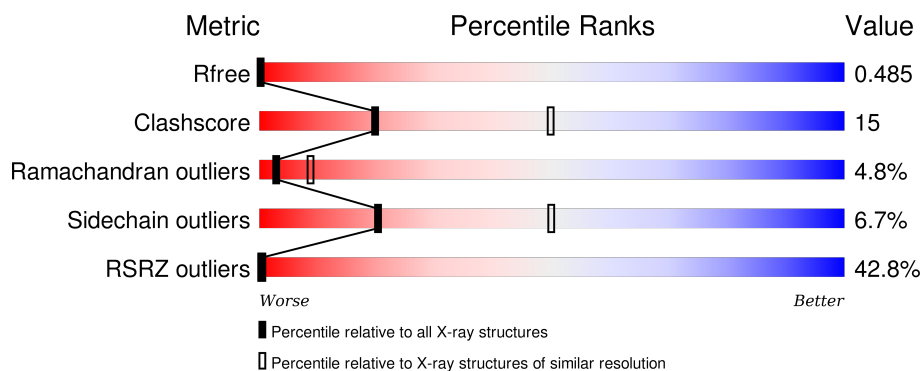
1 Overall quality at a glance

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>27%</div> <div>61% 23% 5% 11%</div> </div>
1	B	300	<div> <div>57%</div> <div>59% 24% 6% 11%</div> </div>
1	C	300	<div> <div>30%</div> <div>61% 27% • 11%</div> </div>

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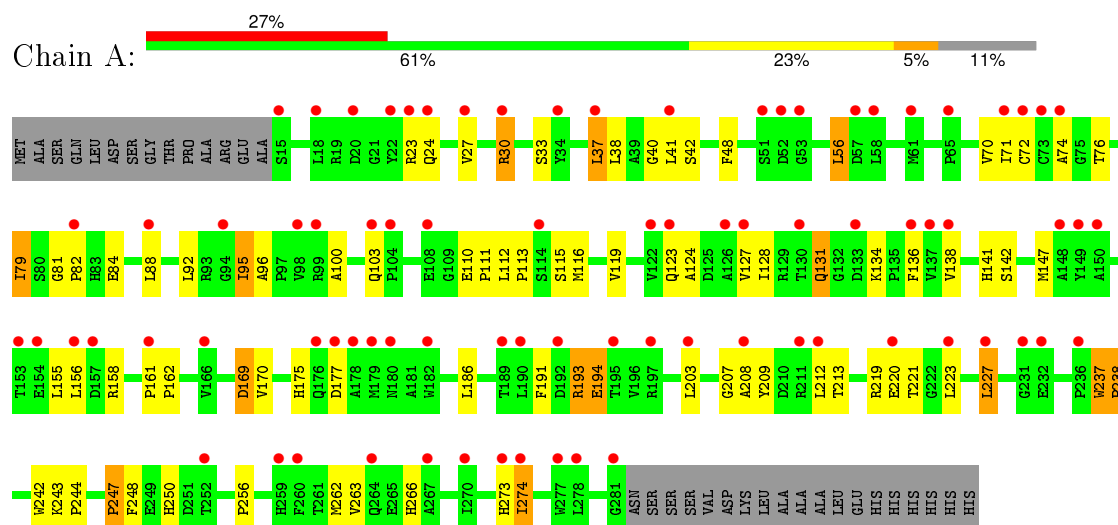
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	217	Total 217	O 217	0	0
2	C	93	Total 93	O 93	0	0

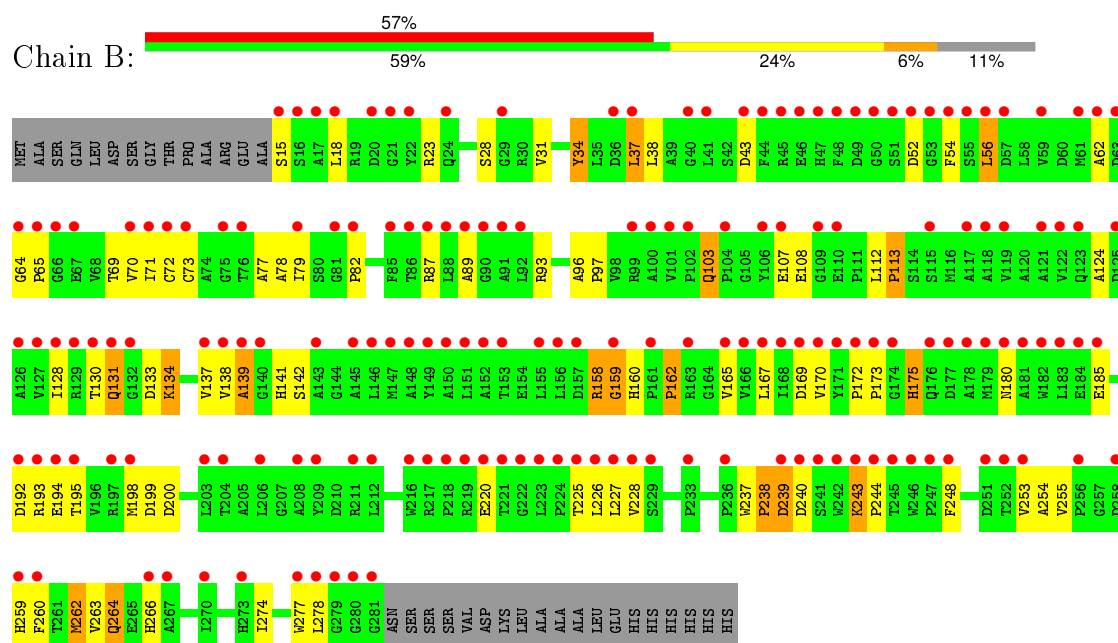
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

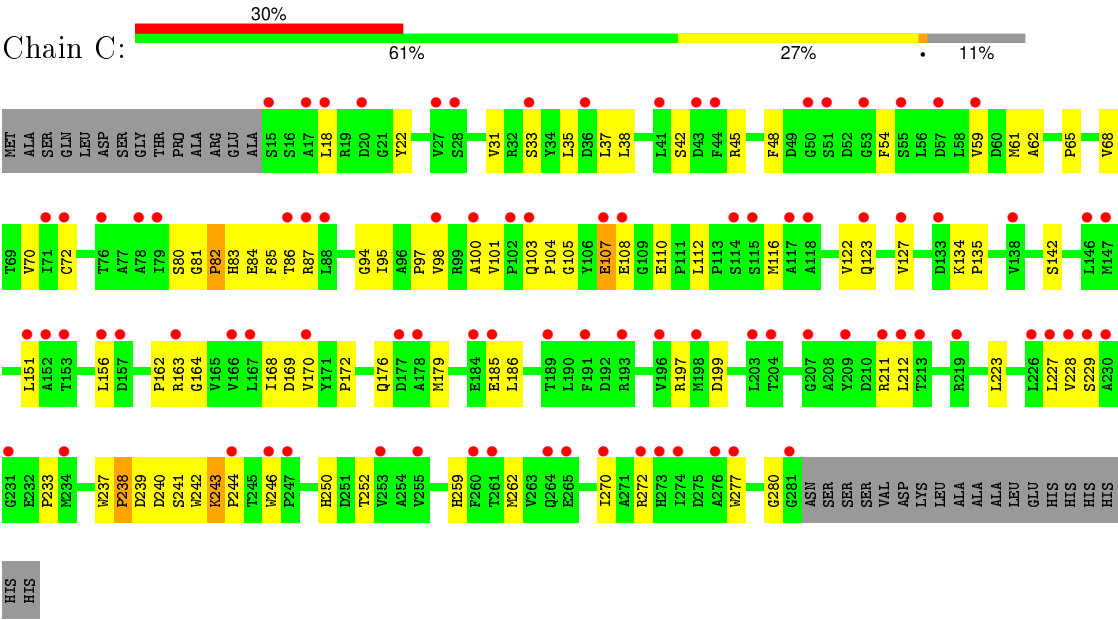
● Molecule 1: ERYTHRONOLIDE SYNTHASE



- 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 49.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.80) 89.6 (49.68-2.80)	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	Depositor
R, R_{free}	0.254 , 0.279 0.474 , 0.485	Depositor DCC
R_{free} test set	2276 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , -10.0	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 50859 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/2065	0.58	0/2821
1	B	0.40	0/2065	0.66	0/2821
1	C	0.35	0/2065	0.58	0/2821
All	All	0.37	0/6195	0.61	0/8463

There are no bond length outliers.

There are no bond angle outliers.

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	64	0
1	B	2011	0	1925	66	0
1	C	2011	0	1925	50	0
2	A	83	0	0	12	0
2	B	217	0	0	26	0
2	C	93	0	0	2	0
All	All	6426	0	5775	176	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 (176) 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: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:A:194:GLU:CD	1:A:194:GLU:H	1.95	0.69
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:107:GLU:HG3	1:C:108:GLU:H	1.60	0.65
1:C:105:GLY:HA2	1:C:110:GLU:O	1.97	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:C:82:PRO:HB3	1:C:100:ALA:HB1	1.80	0.62
1:B:165:VAL:HB	2:B:321:HOH:O	1.98	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: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:B:170:VAL:HG22	2:B:373:HOH:O	2.05	0.56
1:A:88:LEU:HD22	2:A:323: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:119:VAL:HG11	1:A:147:MET:HE1	1.89	0.54
1:C:105:GLY:HA3	1:C:112:LEU:HD23	1.90	0.54
1:A:273:HIS:HB3	2:A:377:HOH:O	2.09	0.53
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:A:76:THR:O	1:A:76:THR:HG22	2.09	0.52
1:C:164:GLY:HA3	1:C:277:TRP:CH2	2.45	0.52
1:C:179:MET:SD	1:C:237:TRP:CZ2	3.03	0.52
1:A:24:GLN:O	1:A:27:VAL:HG22	2.10	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:131:GLN:HE21	1:A:134:LYS:HB3	1.74	0.51
1:A:95:ILE:N	1:A:95:ILE:HD12	2.25	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:68:VAL:HG22	1:C:135:PRO:HB2	1.93	0.51
1:C:33:SER:O	1:C:37:LEU:HD23	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:141:HIS:CE1	1:B:262:MET:SD	3.07	0.48
1:A:124:ALA:HB1	1:A:155:LEU:HD21	1.96	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:123:GLN:O	1:C:127:VAL:HG23	2.15	0.47
1:C:80:SER:O	1:C:83:HIS:NE2	2.48	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:B:65:PRO:O	1:B:96:ALA:HA	2.15	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: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:B:254:ALA:O	1:B:255:VAL:HG23	2.16	0.46
1:A:70:VAL:HG12	1:A:72:CYS:SG	2.56	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:HG22	1:B:128:ILE:O	2.15	0.45
1:C:170:VAL:O	1:C:172:PRO:HD3	2.16	0.45
1:C:164:GLY:HA3	1:C:277:TRP:HH2	1.81	0.45
1:C:81:GLY:O	1:C:84:GLU:HG2	2.15	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
1:C:105:GLY:HA3	1:C:112:LEU:CD2	2.46	0.45
1:C:72:CYS:SG	1:C:98:VAL:HG13	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:59:VAL:HG21	1:C:82:PRO:HB2	2.00	0.44
1:B:23:ARG:HB2	2:B:484:HOH:O	2.17	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:C:48:PHE:HE1	1:C:122:VAL:HG21	1.83	0.43
1:B:31:VAL:HA	2:B:330:HOH:O	2.18	0.43
1:A:116:MET:SD	1:A:213:THR:HG22	2.59	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:124:ALA:HB1	2:B:303:HOH:O	2.20	0.42
1:B:113:PRO:HD2	2:B:316:HOH:O	2.19	0.42
1:C:151:LEU:HD22	2:C:312:HOH:O	2.18	0.42
1:C:172:PRO:HD2	1:C:176:GLN:OE1	2.20	0.42
1:C:54:PHE:HE1	1:C:104:PRO:HB2	1.84	0.42
1:C:134:LYS:HA	1:C:135:PRO:HD3	1.87	0.42
1:B:198:MET:HE3	2:B:331:HOH:O	2.19	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:237:TRP:HA	1:B:238:PRO:HD3	1.85	0.42
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:B:71:ILE:HG22	1:B:72:CYS:H	1.83	0.41
1:A:116:MET:HE1	1:A:213:THR:HG22	2.01	0.41
1:A:81:GLY:O	1:A:84:GLU:HG2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:84:GLU:C	1:C:86:THR:H	2.24	0.41
1:A:156:LEU:HD22	1:A:221:THR:OG1	2.21	0.41
1:B:56:LEU:HD23	1:B:56:LEU:N	2.36	0.40
1:A:237:TRP:HA	1:A:238:PRO:HD3	1.84	0.40
1:C:42:SER:O	1:C:45:ARG:HB2	2.20	0.40
1:B:243:LYS:HA	1:B:244:PRO:HD3	1.87	0.40
1:B:159:GLY:O	1:B:160:HIS:CG	2.75	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 [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	265/300 (88%)	219 (83%)	39 (15%)	7 (3%)	7	22
1	B	265/300 (88%)	189 (71%)	54 (20%)	22 (8%)	1	2
1	C	265/300 (88%)	218 (82%)	38 (14%)	9 (3%)	5	16
All	All	795/900 (88%)	626 (79%)	131 (16%)	38 (5%)	3	9

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

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Mol	Chain	Res	Type
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%)	189 (93%)	15 (7%)	17	43
1	B	204/230 (89%)	187 (92%)	17 (8%)	14	38
1	C	204/230 (89%)	195 (96%)	9 (4%)	35	69
All	All	612/690 (89%)	571 (93%)	41 (7%)	20	50

All (41) 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	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	34	TYR
1	B	37	LEU
1	B	43	ASP
1	B	56	LEU
1	B	103	GLN
1	B	130	THR
1	B	134	LYS
1	B	158	ARG
1	B	175	HIS
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	239	ASP
1	C	87	ARG
1	C	103	GLN

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Mol	Chain	Res	Type
1	C	107	GLU
1	C	186	LEU
1	C	197	ARG
1	C	199	ASP
1	C	211	ARG
1	C	252	THR
1	C	272	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	47	HIS
1	A	131	GLN
1	B	103	GLN
1	B	141	HIS
1	B	264	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	267/300 (89%)	1.68	81 (30%) 1 0	52, 64, 88, 123	0
1	B	267/300 (89%)	3.92	172 (64%) 0 0	32, 68, 76, 83	0
1	C	267/300 (89%)	1.77	90 (33%) 0 0	52, 64, 90, 118	0
All	All	801/900 (89%)	2.46	343 (42%) 0 0	32, 65, 86, 123	0

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	ALA	22.3
1	B	71	ILE	21.7
1	B	167	LEU	18.6
1	B	151	LEU	18.3
1	B	72	CYS	18.2
1	B	152	ALA	17.5
1	B	168	ILE	17.1
1	B	227	LEU	16.2
1	B	226	LEU	15.3
1	B	166	VAL	15.2
1	B	260	PHE	13.0
1	C	281	GLY	11.6
1	B	100	ALA	11.6
1	B	73	CYS	11.5
1	A	15	SER	11.0
1	B	173	PRO	10.5
1	B	174	GLY	10.3
1	B	221	THR	10.2
1	B	51	SER	9.8
1	B	90	GLY	9.7
1	B	89	ALA	9.7
1	B	179	MET	9.5
1	B	212	LEU	9.4

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Mol	Chain	Res	Type	RSRZ
1	B	118	ALA	9.3
1	B	138	VAL	9.0
1	B	244	PRO	9.0
1	A	192	ASP	8.8
1	B	224	PRO	8.6
1	B	127	VAL	8.3
1	C	157	ASP	8.0
1	B	40	GLY	7.9
1	B	165	VAL	7.8
1	B	128	ILE	7.8
1	B	149	TYR	7.5
1	B	37	LEU	7.5
1	B	88	LEU	7.4
1	A	157	ASP	7.3
1	A	20	ASP	7.1
1	B	119	VAL	7.1
1	B	147	MET	7.1
1	B	153	THR	7.1
1	B	163	ARG	7.0
1	B	130	THR	6.9
1	B	228	VAL	6.9
1	B	172	PRO	6.8
1	B	243	LYS	6.8
1	B	150	ALA	6.8
1	B	218	PRO	6.8
1	B	46	GLU	6.7
1	B	220	GLU	6.7
1	B	242	TRP	6.4
1	B	156	LEU	6.3
1	C	189	THR	6.3
1	B	92	LEU	6.1
1	B	117	ALA	6.1
1	B	246	TRP	6.1
1	B	225	THR	6.1
1	C	226	LEU	6.1
1	C	229	SER	6.0
1	B	209	TYR	6.0
1	B	240	ASP	5.9
1	C	264	GLN	5.8
1	B	222	GLY	5.7
1	B	245	THR	5.7
1	B	140	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	197	ARG	5.6
1	B	101	VAL	5.6
1	B	252	THR	5.6
1	B	48	PHE	5.5
1	B	50	GLY	5.5
1	B	146	LEU	5.5
1	A	57	ASP	5.4
1	B	41	LEU	5.4
1	B	56	LEU	5.4
1	B	15	SER	5.4
1	B	121	ALA	5.4
1	B	104	PRO	5.3
1	B	182	TRP	5.3
1	B	193	ARG	5.2
1	B	126	ALA	5.2
1	A	190	LEU	5.1
1	B	170	VAL	5.1
1	B	57	ASP	5.1
1	B	91	ALA	5.1
1	B	178	ALA	5.1
1	A	178	ALA	5.0
1	B	259	HIS	5.0
1	B	122	VAL	5.0
1	C	114	SER	5.0
1	B	66	GLY	4.9
1	B	70	VAL	4.8
1	B	53	GLY	4.7
1	B	52	ASP	4.7
1	A	203	LEU	4.7
1	B	86	THR	4.7
1	B	102	PRO	4.7
1	B	109	GLY	4.6
1	B	217	ARG	4.6
1	B	55	SER	4.6
1	B	211	ARG	4.6
1	C	177	ASP	4.6
1	C	153	THR	4.6
1	B	67	GLU	4.6
1	B	64	GLY	4.6
1	B	131	GLN	4.5
1	B	63	ASP	4.5
1	B	29	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	45	ARG	4.4
1	B	277	TRP	4.4
1	A	126	ALA	4.4
1	A	264	GLN	4.4
1	A	71	ILE	4.3
1	A	133	ASP	4.3
1	B	219	ARG	4.2
1	B	21	GLY	4.2
1	B	281	GLY	4.2
1	B	229	SER	4.1
1	B	123	GLN	4.1
1	A	130	THR	4.1
1	A	108	GLU	4.0
1	C	231	GLY	4.0
1	B	266	HIS	3.9
1	A	227	LEU	3.9
1	B	159	GLY	3.9
1	B	132	GLY	3.9
1	B	236	PRO	3.8
1	B	36	ASP	3.8
1	C	185	GLU	3.8
1	C	102	PRO	3.8
1	A	30	ARG	3.8
1	B	59	VAL	3.8
1	B	280	GLY	3.8
1	A	41	LEU	3.8
1	B	76	THR	3.8
1	C	146	LEU	3.7
1	B	54	PHE	3.7
1	A	195	THR	3.7
1	B	75	GLY	3.7
1	C	163	ARG	3.7
1	B	216	TRP	3.7
1	B	82	PRO	3.7
1	B	267	ALA	3.7
1	C	44	PHE	3.7
1	A	197	ARG	3.7
1	C	270	ILE	3.6
1	B	61	MET	3.6
1	A	27	VAL	3.6
1	B	169	ASP	3.6
1	A	232	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	184	GLU	3.6
1	A	177	ASP	3.6
1	B	185	GLU	3.6
1	B	184	GLU	3.5
1	C	156	LEU	3.5
1	A	138	VAL	3.5
1	A	166	VAL	3.5
1	C	198	MET	3.5
1	C	167	LEU	3.5
1	C	204	THR	3.5
1	B	137	VAL	3.5
1	C	43	ASP	3.4
1	A	220	GLU	3.4
1	A	22	TYR	3.4
1	A	72	CYS	3.4
1	B	65	PRO	3.4
1	B	251	ASP	3.4
1	C	277	TRP	3.4
1	B	177	ASP	3.4
1	A	176	GLN	3.4
1	C	15	SER	3.3
1	B	203	LEU	3.3
1	C	246	TRP	3.3
1	A	88	LEU	3.3
1	B	233	PRO	3.2
1	B	44	PHE	3.2
1	B	99	ARG	3.2
1	A	212	LEU	3.2
1	C	79	ILE	3.2
1	C	230	ALA	3.2
1	A	277	TRP	3.2
1	A	149	TYR	3.2
1	B	273	HIS	3.2
1	A	82	PRO	3.1
1	A	104	PRO	3.1
1	C	76	THR	3.1
1	B	248	PHE	3.1
1	A	273	HIS	3.1
1	C	261	THR	3.1
1	B	194	GLU	3.1
1	A	98	VAL	3.1
1	C	152	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	171	TYR	3.0
1	C	196	VAL	3.0
1	C	59	VAL	3.0
1	C	247	PRO	3.0
1	A	99	ARG	3.0
1	C	228	VAL	3.0
1	B	183	LEU	3.0
1	A	179	MET	3.0
1	B	198	MET	3.0
1	A	211	ARG	3.0
1	C	36	ASP	3.0
1	B	85	PHE	3.0
1	B	79	ILE	2.9
1	A	208	ALA	2.9
1	B	204	THR	2.9
1	B	270	ILE	2.9
1	C	41	LEU	2.9
1	B	143	ALA	2.9
1	B	43	ASP	2.9
1	B	49	ASP	2.9
1	B	247	PRO	2.9
1	B	148	ALA	2.9
1	A	153	THR	2.9
1	C	151	LEU	2.9
1	C	108	GLU	2.9
1	C	260	PHE	2.9
1	C	273	HIS	2.9
1	B	279	GLY	2.9
1	B	115	SER	2.9
1	C	274	ILE	2.9
1	C	193	ARG	2.9
1	C	166	VAL	2.8
1	B	256	PRO	2.8
1	C	51	SER	2.8
1	B	129	ARG	2.8
1	C	272	ARG	2.8
1	B	155	LEU	2.8
1	C	234	MET	2.8
1	C	207	GLY	2.8
1	B	24	GLN	2.8
1	B	241	SER	2.8
1	A	148	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	78	ALA	2.8
1	C	127	VAL	2.8
1	C	28	SER	2.7
1	A	122	VAL	2.7
1	C	244	PRO	2.7
1	C	123	GLN	2.7
1	C	133	ASP	2.7
1	C	86	THR	2.7
1	C	98	VAL	2.7
1	C	27	VAL	2.7
1	B	239	ASP	2.7
1	C	115	SER	2.7
1	B	208	ALA	2.7
1	A	156	LEU	2.7
1	C	203	LEU	2.7
1	C	55	SER	2.7
1	A	24	GLN	2.7
1	A	161	PRO	2.7
1	A	18	LEU	2.7
1	A	270	ILE	2.6
1	B	17	ALA	2.6
1	B	22	TYR	2.6
1	B	181	ALA	2.6
1	C	191	PHE	2.6
1	C	147	MET	2.6
1	A	74	ALA	2.6
1	A	123	GLN	2.6
1	B	157	ASP	2.6
1	C	72	CYS	2.6
1	C	18	LEU	2.6
1	B	62	ALA	2.6
1	A	34	TYR	2.6
1	A	52	ASP	2.6
1	B	20	ASP	2.6
1	C	87	ARG	2.5
1	A	58	LEU	2.5
1	B	206	LEU	2.5
1	A	23	ARG	2.5
1	C	33	SER	2.5
1	C	211	ARG	2.5
1	A	150	ALA	2.5
1	A	260	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	219	ARG	2.4
1	C	107	GLU	2.4
1	A	114	SER	2.4
1	C	209	TYR	2.4
1	C	57	ASP	2.4
1	B	18	LEU	2.4
1	A	65	PRO	2.4
1	A	53	GLY	2.4
1	B	16	SER	2.4
1	C	71	ILE	2.4
1	C	100	ALA	2.4
1	A	180	ASN	2.4
1	B	195	THR	2.4
1	C	138	VAL	2.4
1	A	137	VAL	2.4
1	A	189	THR	2.4
1	B	192	ASP	2.4
1	B	258	ASP	2.4
1	C	53	GLY	2.3
1	A	274	ILE	2.3
1	B	110	GLU	2.3
1	B	145	ALA	2.3
1	C	17	ALA	2.3
1	A	73	CYS	2.3
1	A	236	PRO	2.3
1	A	281	GLY	2.3
1	B	87	ARG	2.3
1	A	37	LEU	2.3
1	A	103	GLN	2.3
1	A	278	LEU	2.3
1	A	94	GLY	2.2
1	C	255	VAL	2.2
1	B	176	GLN	2.2
1	B	107	GLU	2.2
1	C	178	ALA	2.2
1	B	47	HIS	2.2
1	A	154	GLU	2.2
1	C	50	GLY	2.2
1	A	127	VAL	2.2
1	C	170	VAL	2.2
1	A	223	LEU	2.2
1	B	278	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	182	TRP	2.2
1	A	231	GLY	2.2
1	A	267	ALA	2.2
1	B	106	TYR	2.2
1	C	20	ASP	2.2
1	C	88	LEU	2.1
1	A	51	SER	2.1
1	B	161	PRO	2.1
1	C	103	GLN	2.1
1	A	61	MET	2.1
1	C	213	THR	2.1
1	B	125	ASP	2.1
1	C	265	GLU	2.1
1	B	253	VAL	2.0
1	C	117	ALA	2.0
1	C	118	ALA	2.0
1	C	276	ALA	2.0
1	C	253	VAL	2.0
1	B	180	ASN	2.0
1	C	227	LEU	2.0
1	A	136	PHE	2.0
1	B	81	GLY	2.0
1	A	259	HIS	2.0
1	A	252	THR	2.0
1	B	223	LEU	2.0
1	C	212	LEU	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 [i](#)

There are no such residues in this entry.