Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:17 pm BST

PDB ID	:	1MNQ
Title	:	Thioesterase Domain of Picromycin Polyketide Synthase (PICS TE), pH 8.4
Authors	:	Tsai, S.-C.; Lu, H.; Cane, D.E.; Khosla, C.; Stroud, R.M.
Deposited on	:	2002-09-05
Resolution	:	2.20 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 following versions of software and data (see references ①) were used in the production of this report:

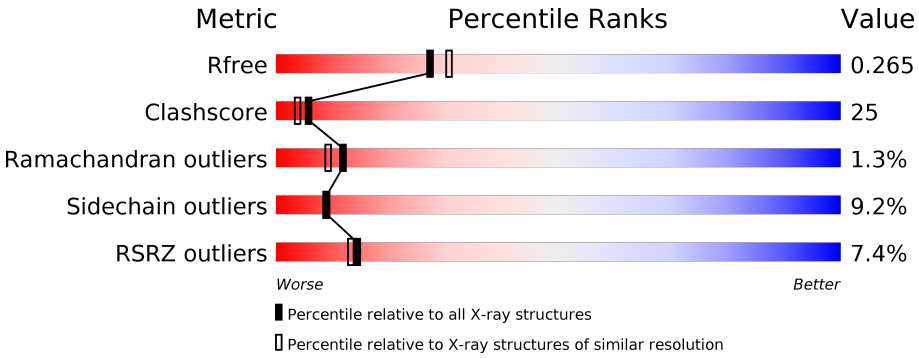
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	298	6% 61% 24% 5% • 8%
1	B	298	7% 63% 23% 5% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4523 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 polyketide synthase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2083	1316	375	385	7			
1	B	277	Total	C	N	O	S	0	0	0
			2100	1327	377	389	7			

- Molecule 2 is water.

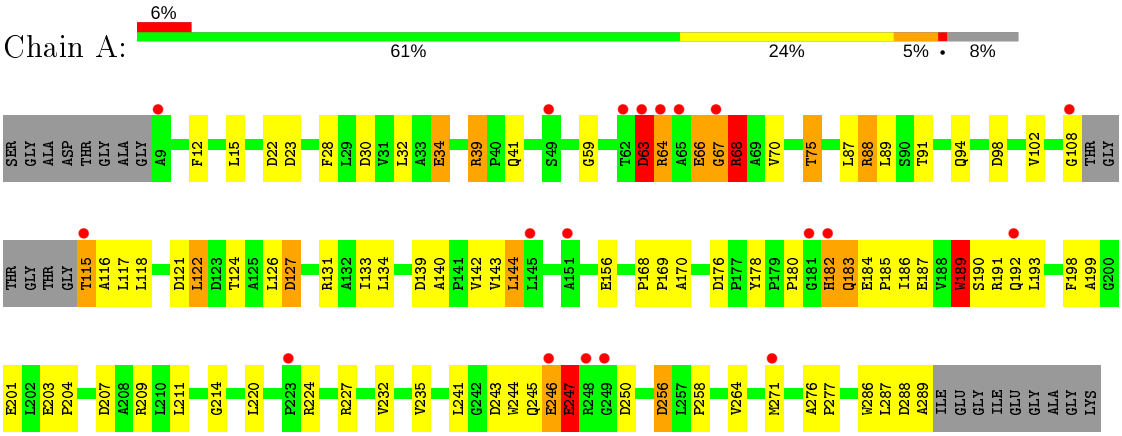
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total	O	0	0
			150	150		
2	B	190	Total	O	0	0
			190	190		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

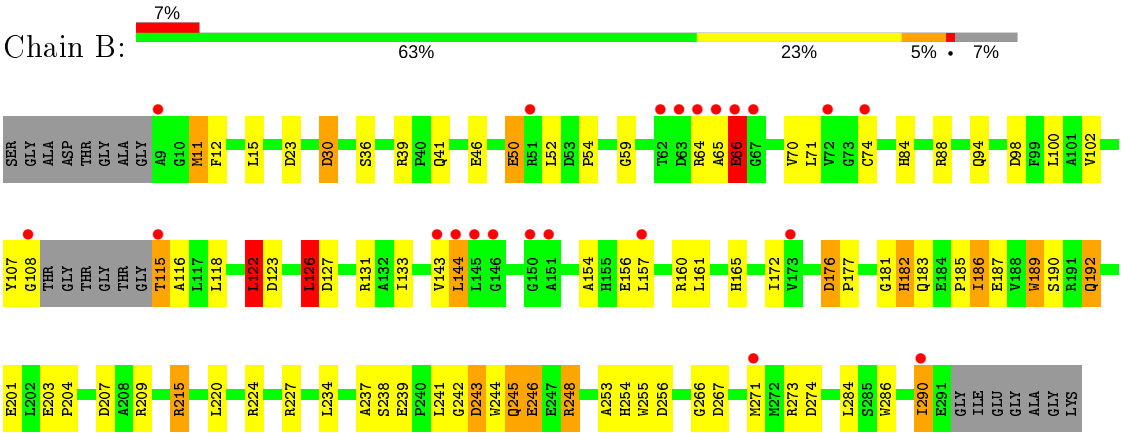
- Molecule 1: polyketide synthase IV

Chain A:



- Molecule 1: polyketide synthase IV

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.02Å 106.22Å 114.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 26.22 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.20) 91.6 (26.22-2.36)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.36Å)	Xtriage
Refinement program	CNS, REFMAC 5.0	Depositor
R, R_{free}	0.220 , 0.248 0.245 , 0.265	Depositor DCC
R_{free} test set	1364 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4523	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.73	0/2139	0.97	15/2916 (0.5%)
1	B	0.86	0/2156	1.07	14/2939 (0.5%)
All	All	0.79	0/4295	1.02	29/5855 (0.5%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ARG	NE-CZ-NH2	-16.26	112.17	120.30
1	B	215	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	B	243	ASP	CB-CG-OD2	8.25	125.72	118.30
1	A	23	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	207	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	288	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	215	ARG	CG-CD-NE	-6.48	98.19	111.80
1	A	189	TRP	CB-CA-C	-6.42	97.56	110.40
1	A	30	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	30	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	22	ASP	CB-CG-OD2	6.03	123.72	118.30
1	B	126	LEU	CB-CG-CD1	5.96	121.13	111.00
1	B	122	LEU	CB-CG-CD2	5.92	121.07	111.00
1	A	39	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	176	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	63	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	39	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	139	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	256	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	127	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	250	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	215	ARG	CD-NE-CZ	5.39	131.15	123.60
1	A	199	ALA	C-N-CA	-5.32	111.13	122.30
1	A	256	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	189	TRP	CA-CB-CG	5.26	123.69	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	189	TRP	CB-CA-C	-5.18	100.04	110.40
1	B	172	ILE	CG1-CB-CG2	-5.08	100.23	111.40
1	B	23	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	98	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2083	0	2011	104	0
1	B	2100	0	2028	106	0
2	A	150	0	0	26	0
2	B	190	0	0	36	0
All	All	4523	0	4039	209	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 25.

All (209) 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:237:ALA:HA	1:B:271:MET:SD	1.56	1.44
1:A:183:GLN:CG	1:A:183:GLN:O	1.72	1.34
1:A:235:VAL:HG12	1:A:271:MET:CE	1.71	1.20
1:B:237:ALA:CA	1:B:271:MET:SD	2.32	1.15
1:B:65:ALA:N	1:B:66:GLU:OE1	1.81	1.13
1:A:191:ARG:HH21	1:A:192:GLN:HG2	1.05	1.11
1:B:244:TRP:O	1:B:245:GLN:HB3	1.36	1.09
1:B:84:HIS:HB2	2:B:363:HOH:O	1.54	1.08
1:A:235:VAL:HG12	1:A:271:MET:HE1	1.15	1.07
1:A:182:HIS:CD2	1:A:182:HIS:O	2.07	1.07
1:B:244:TRP:O	1:B:245:GLN:CB	2.00	1.03
1:A:192:GLN:NE2	1:A:241:LEU:HG	1.72	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLN:HE21	1:A:241:LEU:HG	1.17	1.03
1:A:140:ALA:HB1	2:A:365:HOH:O	1.59	1.00
1:A:63:ASP:HB3	1:A:64:ARG:HH11	1.26	1.00
1:A:32:LEU:HB3	2:A:369:HOH:O	1.60	1.00
1:A:191:ARG:NH2	1:A:192:GLN:HG2	1.76	0.99
1:A:121:ASP:OD1	1:A:124:THR:HG23	1.65	0.97
1:B:107:TYR:O	1:B:108:GLY:O	1.80	0.96
1:B:237:ALA:HB2	1:B:271:MET:HE2	1.47	0.96
1:A:264:VAL:HG22	1:A:271:MET:HE3	1.44	0.95
1:B:123:ASP:HA	2:B:488:HOH:O	1.66	0.94
1:A:88:ARG:HD3	2:A:303:HOH:O	1.67	0.93
1:B:108:GLY:HA3	1:B:209:ARG:HH21	1.31	0.93
1:A:12:PHE:HA	2:A:414:HOH:O	1.69	0.91
1:B:267:ASP:O	1:B:271:MET:HG3	1.70	0.90
1:A:191:ARG:HH21	1:A:192:GLN:CG	1.85	0.90
1:A:15:LEU:HD12	2:A:414:HOH:O	1.72	0.89
1:A:108:GLY:HA2	1:A:209:ARG:HH21	1.38	0.89
1:A:185:PRO:HD2	2:A:361:HOH:O	1.71	0.88
1:B:237:ALA:HB2	1:B:271:MET:CE	2.04	0.88
1:B:177:PRO:HG2	2:B:474:HOH:O	1.73	0.87
1:A:201:GLU:HB3	2:A:311:HOH:O	1.75	0.86
1:A:182:HIS:HD2	1:A:182:HIS:O	1.54	0.86
1:A:191:ARG:NH2	1:A:192:GLN:CG	2.41	0.82
1:A:63:ASP:CB	1:A:64:ARG:HH11	1.93	0.82
1:A:115:THR:OG1	1:A:115:THR:O	1.91	0.82
1:B:183:GLN:HG2	2:B:411:HOH:O	1.78	0.81
1:A:235:VAL:CG1	1:A:271:MET:HE1	2.08	0.79
1:A:63:ASP:HB3	1:A:64:ARG:NH1	1.99	0.78
1:A:227:ARG:HH22	1:A:256:ASP:HB2	1.47	0.78
1:B:154:ALA:HA	2:B:471:HOH:O	1.83	0.78
1:B:156:GLU:HB3	1:B:224:ARG:HH12	1.48	0.77
1:A:235:VAL:CG1	1:A:271:MET:CE	2.60	0.77
1:B:66:GLU:CD	1:B:66:GLU:N	2.38	0.77
1:B:108:GLY:CA	1:B:209:ARG:HH21	1.98	0.77
1:A:183:GLN:HG2	1:A:183:GLN:O	0.79	0.77
1:B:237:ALA:CB	1:B:271:MET:SD	2.73	0.76
1:A:264:VAL:CG2	1:A:271:MET:HE3	2.15	0.75
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.51	0.74
1:B:246:GLU:HB3	2:B:331:HOH:O	1.87	0.74
1:B:234:LEU:HD11	2:B:474:HOH:O	1.88	0.73
1:B:239:GLU:HG3	2:B:392:HOH:O	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLY:H	1:A:94:GLN:HE22	1.34	0.73
1:B:156:GLU:HB3	1:B:224:ARG:NH1	2.04	0.72
1:A:64:ARG:HD3	1:A:64:ARG:H	1.54	0.71
1:A:116:ALA:HB1	2:A:326:HOH:O	1.90	0.70
1:B:107:TYR:O	1:B:108:GLY:C	2.26	0.69
1:A:189:TRP:CZ3	1:A:243:ASP:O	2.47	0.67
1:B:65:ALA:C	1:B:66:GLU:OE1	2.33	0.67
1:A:264:VAL:CG2	1:A:271:MET:CE	2.71	0.67
1:B:108:GLY:H	1:B:209:ARG:HE	1.42	0.67
1:A:227:ARG:NH2	1:A:256:ASP:HB2	2.12	0.65
1:B:127:ASP:HA	2:B:379:HOH:O	1.96	0.65
1:A:66:GLU:OE1	1:A:67:GLY:N	2.30	0.65
1:A:108:GLY:CA	1:A:209:ARG:HH21	2.10	0.65
1:B:244:TRP:CZ2	1:B:248:ARG:HG3	2.32	0.65
1:A:214:GLY:HA3	2:A:369:HOH:O	1.96	0.65
1:A:89:LEU:HD11	2:A:420:HOH:O	1.97	0.64
1:B:239:GLU:HG2	2:B:466:HOH:O	1.97	0.64
1:A:178:TYR:CD1	1:A:186:ILE:HD12	2.32	0.63
1:A:286:TRP:HA	2:A:426:HOH:O	1.98	0.63
1:B:192:GLN:HG3	2:B:450:HOH:O	1.99	0.63
1:B:30:ASP:HB3	2:B:390:HOH:O	1.98	0.63
1:A:264:VAL:HG22	1:A:271:MET:CE	2.23	0.63
1:A:64:ARG:N	1:A:64:ARG:HD3	2.13	0.63
1:B:266:GLY:N	2:B:466:HOH:O	2.32	0.62
1:A:211:LEU:HA	2:A:369:HOH:O	1.98	0.62
1:B:144:LEU:HG	2:B:471:HOH:O	1.98	0.62
1:B:248:ARG:HB2	2:B:339:HOH:O	1.99	0.62
1:B:41:GLN:HB2	1:B:118:LEU:O	2.00	0.62
1:B:165:HIS:NE2	2:B:379:HOH:O	2.26	0.61
1:B:201:GLU:HB2	1:B:203:GLU:O	2.00	0.61
1:B:203:GLU:HB2	1:B:204:PRO:HD2	1.83	0.61
1:A:59:GLY:H	1:A:94:GLN:NE2	1.98	0.60
1:A:189:TRP:HZ3	1:A:243:ASP:O	1.84	0.60
1:A:75:THR:HG23	1:A:102:VAL:O	2.01	0.60
1:A:142:VAL:C	2:A:355:HOH:O	2.41	0.59
1:B:64:ARG:C	1:B:66:GLU:OE1	2.41	0.59
1:A:192:GLN:HE22	1:A:241:LEU:C	2.05	0.59
1:B:237:ALA:CB	1:B:271:MET:CE	2.80	0.58
1:A:68:ARG:CG	1:A:68:ARG:HH11	2.14	0.58
1:A:70:VAL:HG23	2:A:365:HOH:O	2.03	0.58
1:B:66:GLU:OE1	1:B:66:GLU:N	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:HH22	1:A:256:ASP:CB	2.15	0.58
1:A:232:VAL:CG2	1:A:258:PRO:HA	2.34	0.57
1:B:181:GLY:O	1:B:182:HIS:CB	2.49	0.57
1:A:156:GLU:OE1	1:A:224:ARG:HD3	2.05	0.57
1:B:286:TRP:O	1:B:290:ILE:HD13	2.04	0.57
1:A:108:GLY:H	1:A:209:ARG:HE	1.52	0.57
1:B:238:SER:HB2	2:B:466:HOH:O	2.04	0.56
1:B:71:LEU:HD23	1:B:143:VAL:HG13	1.86	0.56
1:A:75:THR:CG2	1:A:102:VAL:O	2.54	0.56
1:B:237:ALA:HB2	1:B:271:MET:SD	2.44	0.56
1:B:102:VAL:HG11	1:B:133:ILE:CG1	2.35	0.56
1:A:39:ARG:HD3	2:A:359:HOH:O	2.05	0.56
1:B:241:LEU:HB3	2:B:450:HOH:O	2.05	0.56
1:A:201:GLU:HB2	1:A:203:GLU:O	2.06	0.55
1:A:182:HIS:HA	2:A:353:HOH:O	2.05	0.55
1:B:237:ALA:N	1:B:271:MET:HE1	2.22	0.55
1:A:184:GLU:N	1:A:185:PRO:CD	2.70	0.55
1:B:65:ALA:CA	1:B:66:GLU:OE1	2.54	0.54
1:B:227:ARG:HG2	1:B:227:ARG:HH11	1.72	0.54
1:B:254:HIS:N	2:B:474:HOH:O	2.40	0.54
1:A:264:VAL:HG21	1:A:271:MET:HE2	1.90	0.54
1:B:253:ALA:HB1	2:B:474:HOH:O	2.06	0.54
1:B:160:ARG:HD3	2:B:488:HOH:O	2.08	0.54
1:A:28:PHE:HZ	2:A:414:HOH:O	1.91	0.53
1:A:189:TRP:CH2	1:A:243:ASP:O	2.61	0.53
1:B:246:GLU:CA	1:B:246:GLU:OE1	2.57	0.53
1:B:183:GLN:O	1:B:186:ILE:HG22	2.08	0.53
1:B:39:ARG:HD3	2:B:385:HOH:O	2.09	0.53
1:A:224:ARG:NH2	2:A:320:HOH:O	2.41	0.53
1:A:235:VAL:HG12	1:A:271:MET:HE2	1.79	0.53
1:B:189:TRP:CZ3	1:B:243:ASP:O	2.63	0.52
1:B:182:HIS:CG	2:B:384:HOH:O	2.61	0.52
1:B:183:GLN:NE2	2:B:460:HOH:O	2.39	0.52
1:A:185:PRO:CD	2:A:361:HOH:O	2.40	0.52
1:B:189:TRP:CH2	1:B:242:GLY:O	2.64	0.51
1:B:237:ALA:CA	1:B:271:MET:CE	2.89	0.51
1:B:115:THR:HG22	1:B:116:ALA:N	2.26	0.51
1:B:41:GLN:CB	1:B:118:LEU:O	2.59	0.51
1:A:264:VAL:HG21	1:A:271:MET:CE	2.40	0.51
1:B:227:ARG:NH2	1:B:255:TRP:CZ2	2.79	0.50
1:B:36:SER:OG	1:B:215:ARG:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:TRP:NE1	1:B:290:ILE:HD11	2.27	0.49
1:A:180:PRO:C	1:A:182:HIS:H	2.15	0.49
1:B:122:LEU:HD13	1:B:224:ARG:NH1	2.27	0.49
1:B:54:PRO:HG3	1:B:102:VAL:HG12	1.95	0.49
1:B:131:ARG:NH2	2:B:476:HOH:O	2.45	0.49
1:B:181:GLY:O	1:B:182:HIS:HB3	2.13	0.49
1:B:126:LEU:HD23	2:B:488:HOH:O	2.14	0.48
1:A:68:ARG:NH1	1:A:68:ARG:CG	2.71	0.48
1:B:102:VAL:HG11	1:B:133:ILE:HG12	1.95	0.48
1:A:276:ALA:N	1:A:277:PRO:CD	2.76	0.48
1:A:189:TRP:CD1	1:A:241:LEU:HB3	2.49	0.47
1:A:264:VAL:HG21	1:A:271:MET:HG3	1.96	0.47
1:A:235:VAL:CG1	1:A:271:MET:HE2	2.40	0.47
1:A:170:ALA:HA	2:A:416:HOH:O	2.14	0.47
1:A:63:ASP:HB3	1:A:64:ARG:HD3	1.97	0.46
1:B:122:LEU:CD1	1:B:224:ARG:NH1	2.78	0.46
1:B:182:HIS:N	1:B:182:HIS:ND1	2.63	0.46
1:A:178:TYR:HB3	1:A:183:GLN:HB2	1.97	0.46
1:A:68:ARG:N	2:A:367:HOH:O	2.47	0.46
1:B:189:TRP:HZ3	1:B:243:ASP:O	1.99	0.46
1:B:245:GLN:HG2	2:B:429:HOH:O	2.16	0.46
1:B:286:TRP:CD1	1:B:290:ILE:HD11	2.51	0.46
1:A:144:LEU:N	1:A:144:LEU:CD1	2.79	0.45
1:B:126:LEU:CD2	2:B:488:HOH:O	2.65	0.45
1:A:168:PRO:HA	1:A:169:PRO:HD2	1.90	0.45
1:A:203:GLU:HB2	1:A:204:PRO:HD2	1.98	0.45
1:B:227:ARG:NH1	1:B:227:ARG:HG2	2.30	0.45
1:B:11:MET:HA	1:B:11:MET:HE2	1.99	0.45
1:B:182:HIS:N	1:B:182:HIS:HD1	2.15	0.45
1:A:70:VAL:HG22	1:A:98:ASP:HB2	1.99	0.44
1:B:59:GLY:H	1:B:94:GLN:HE22	1.65	0.44
1:B:237:ALA:N	1:B:271:MET:SD	2.88	0.44
1:A:39:ARG:HG2	1:B:15:LEU:HD21	1.99	0.44
1:B:50:GLU:HG3	1:B:52:LEU:HD21	1.99	0.44
1:B:71:LEU:HA	1:B:143:VAL:HG13	1.99	0.44
1:B:88:ARG:HD2	1:B:273:ARG:HA	1.99	0.44
1:A:245:GLN:C	1:A:247:GLU:N	2.71	0.44
1:A:183:GLN:C	2:A:361:HOH:O	2.56	0.44
1:B:127:ASP:OD1	2:B:379:HOH:O	2.21	0.44
1:B:12:PHE:HB2	1:B:207:ASP:CG	2.39	0.44
1:A:185:PRO:N	2:A:361:HOH:O	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:HG3	2:A:417:HOH:O	2.17	0.43
1:B:156:GLU:HG3	1:B:224:ARG:HH11	1.83	0.43
1:A:41:GLN:CB	1:A:118:LEU:O	2.66	0.43
1:A:122:LEU:HD22	1:A:126:LEU:HG	2.00	0.43
1:A:198:PHE:HA	2:A:311:HOH:O	2.18	0.43
1:B:183:GLN:CG	2:B:411:HOH:O	2.52	0.43
1:B:237:ALA:N	1:B:271:MET:CE	2.81	0.43
1:A:127:ASP:O	1:A:131:ARG:HG3	2.19	0.43
1:A:34:GLU:OE1	1:A:34:GLU:HA	2.18	0.43
1:B:273:ARG:HB2	1:B:274:ASP:H	1.50	0.43
1:A:180:PRO:C	1:A:182:HIS:N	2.72	0.43
1:A:63:ASP:CB	1:A:64:ARG:NH1	2.69	0.42
1:B:290:ILE:CD1	1:B:290:ILE:N	2.81	0.42
1:B:70:VAL:HB	2:B:446:HOH:O	2.18	0.42
1:A:170:ALA:HB3	2:A:355:HOH:O	2.19	0.42
1:A:287:LEU:O	1:A:289:ALA:N	2.52	0.42
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.77	0.42
1:A:88:ARG:HB2	1:A:88:ARG:HE	1.60	0.42
1:B:74:CYS:SG	2:B:471:HOH:O	2.61	0.42
1:B:241:LEU:CB	2:B:450:HOH:O	2.65	0.42
1:B:156:GLU:CG	1:B:224:ARG:HH11	2.33	0.42
1:B:100:LEU:HG	2:B:446:HOH:O	2.20	0.41
1:B:284:LEU:HA	1:B:284:LEU:HD23	1.79	0.41
1:A:68:ARG:HG2	1:A:68:ARG:NH1	2.27	0.41
1:A:189:TRP:HH2	1:A:244:TRP:HB2	1.86	0.41
1:B:185:PRO:HA	1:B:244:TRP:CZ3	2.56	0.41
1:A:66:GLU:O	1:A:67:GLY:C	2.57	0.41
1:B:46:GLU:HB3	1:B:131:ARG:HH12	1.85	0.41
1:A:186:ILE:HG12	1:A:193:LEU:HD11	2.03	0.40
1:A:102:VAL:HG21	1:A:133:ILE:HG12	2.02	0.40
1:B:187:GLU:O	1:B:190:SER:HB2	2.22	0.40
1:B:157:LEU:HB3	2:B:471:HOH:O	2.19	0.40
1:B:182:HIS:HA	2:B:401:HOH:O	2.21	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	271/298 (91%)	253 (93%)	13 (5%)	5 (2%)	8 5
1	B	273/298 (92%)	263 (96%)	8 (3%)	2 (1%)	22 22
All	All	544/596 (91%)	516 (95%)	21 (4%)	7 (1%)	12 9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	B	66	GLU
1	A	67	GLY
1	A	68	ARG
1	A	246	GLU
1	A	247	GLU
1	B	245	GLN

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	205/216 (95%)	183 (89%)	22 (11%)	6 6
1	B	207/216 (96%)	191 (92%)	16 (8%)	13 13
All	All	412/432 (95%)	374 (91%)	38 (9%)	9 9

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	64	ARG
1	A	66	GLU
1	A	68	ARG
1	A	75	THR
1	A	87	LEU
1	A	88	ARG
1	A	91	THR
1	A	115	THR
1	A	117	LEU
1	A	122	LEU
1	A	143	VAL
1	A	144	LEU
1	A	176	ASP
1	A	182	HIS
1	A	183	GLN
1	A	187	GLU
1	A	189	TRP
1	A	190	SER
1	A	220	LEU
1	A	246	GLU
1	A	247	GLU
1	B	11	MET
1	B	50	GLU
1	B	66	GLU
1	B	115	THR
1	B	122	LEU
1	B	126	LEU
1	B	144	LEU
1	B	161	LEU
1	B	176	ASP
1	B	182	HIS
1	B	186	ILE
1	B	192	GLN
1	B	220	LEU
1	B	246	GLU
1	B	248	ARG
1	B	290	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	182	HIS
1	A	192	GLN
1	B	94	GLN
1	B	147	HIS
1	B	245	GLN
1	B	254	HIS

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, 95^{th} 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	275/298 (92%)	0.35	19 (6%)	16	15	27, 36, 47, 52	0
1	B	277/298 (92%)	0.30	22 (7%)	12	11	28, 36, 48, 57	0
All	All	552/596 (92%)	0.33	41 (7%)	14	13	27, 36, 48, 57	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	ALA	7.9
1	A	65	ALA	6.4
1	B	62	THR	6.3
1	B	64	ARG	5.6
1	A	248	ARG	5.0
1	A	67	GLY	4.8
1	A	9	ALA	4.8
1	B	9	ALA	4.8
1	B	271	MET	4.7
1	A	115	THR	4.6
1	A	62	THR	4.1
1	A	63	ASP	4.1
1	B	108	GLY	3.8
1	A	49	SER	3.8
1	A	108	GLY	3.7
1	A	64	ARG	3.7
1	A	181	GLY	3.7
1	B	63	ASP	3.4
1	A	246	GLU	3.3
1	B	145	LEU	3.3
1	B	115	THR	3.1
1	A	249	GLY	2.9
1	B	51	ARG	2.7
1	B	66	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	151	ALA	2.7
1	B	290	ILE	2.6
1	B	72	VAL	2.6
1	B	74	CYS	2.5
1	B	144	LEU	2.5
1	B	146	GLY	2.5
1	B	173	VAL	2.4
1	B	151	ALA	2.4
1	A	271	MET	2.3
1	A	145	LEU	2.3
1	B	67	GLY	2.3
1	A	182	HIS	2.2
1	B	150	GLY	2.2
1	B	143	VAL	2.1
1	A	223	PRO	2.1
1	B	157	LEU	2.1
1	A	192	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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.