Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 11:25 PM JST

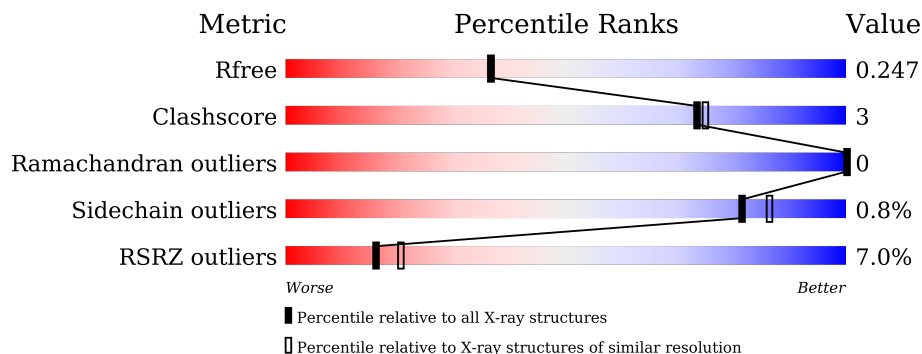|		
PDB ID	:	6K8N
Title	:	Crystal structure of the Sulfolobus solfataricus topoisomerase III
Authors	:	Wang, H.Q.; Zhang, J.H.; Zheng, X.; Zheng, Z.F.; Dong, Y.H.; Huang, L.; Gong, Y.
Deposited on	:	2019-06-13
Resolution	:	2.10 Å(reported)

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 2.10 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		7.0%

Worse ← → Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	668	2% / 91% / 9%
1	B	668	9% / 90% / 9%
1	C	668	8% / 88% / 11%
1	D	668	9% / 91% / 8%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 22583 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 topoisomerase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	668	Total 5401	C 3498	N 908	O 980	S 15	0	0	0
1	B	665	Total 5380	C 3487	N 905	O 973	S 15	0	0	0
1	C	667	Total 5392	C 3493	N 907	O 977	S 15	0	0	0
1	D	666	Total 5386	C 3490	N 906	O 975	S 15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	PHE	TYR	engineered mutation	UNP Q97ZJ8
B	318	PHE	TYR	engineered mutation	UNP Q97ZJ8
C	318	PHE	TYR	engineered mutation	UNP Q97ZJ8
D	318	PHE	TYR	engineered mutation	UNP Q97ZJ8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	323	Total 323	O 323	0	0
3	B	344	Total 344	O 344	0	0
3	C	171	Total 171	O 171	0	0
3	D	182	Total 182	O 182	0	0

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.
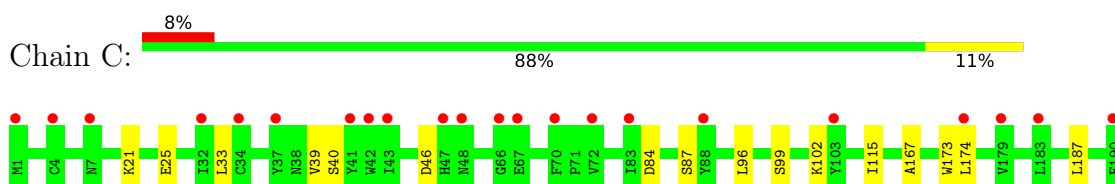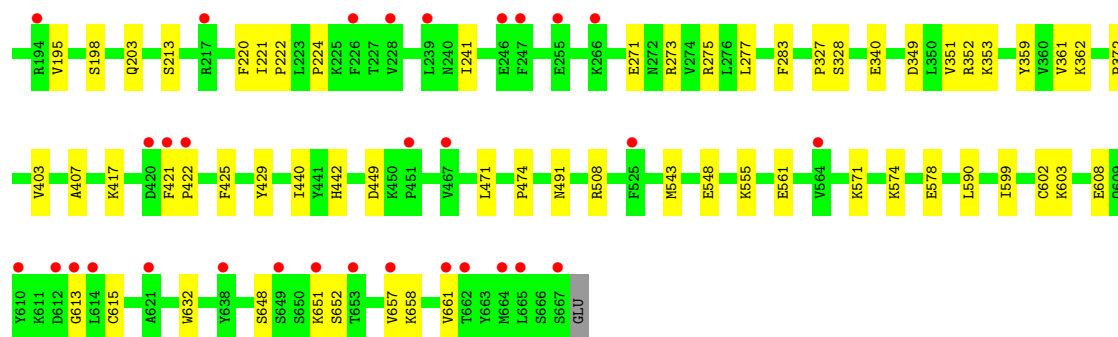
• Molecule 1: topoisomerase III

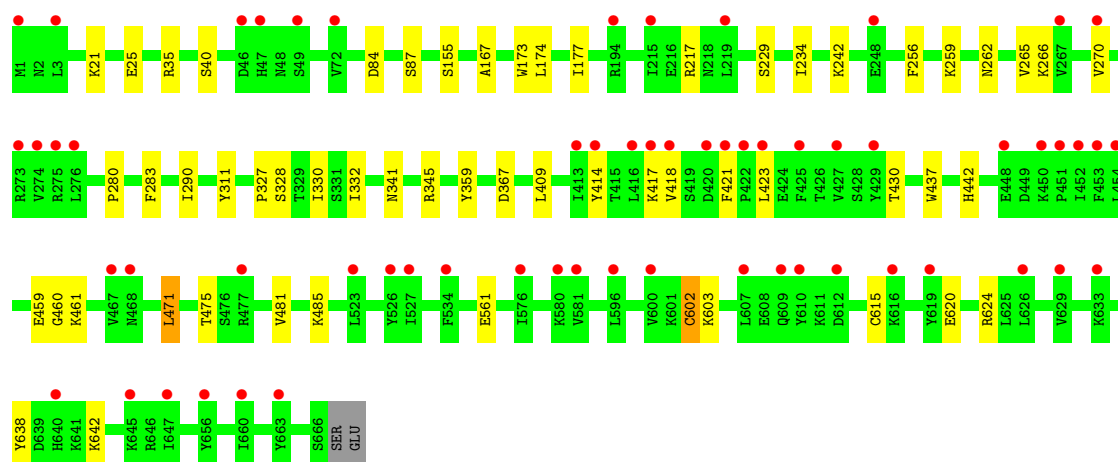Chain A:

• Molecule 1: topoisomerase III

Chain B:

• Molecule 1: topoisomerase III

Chain C:
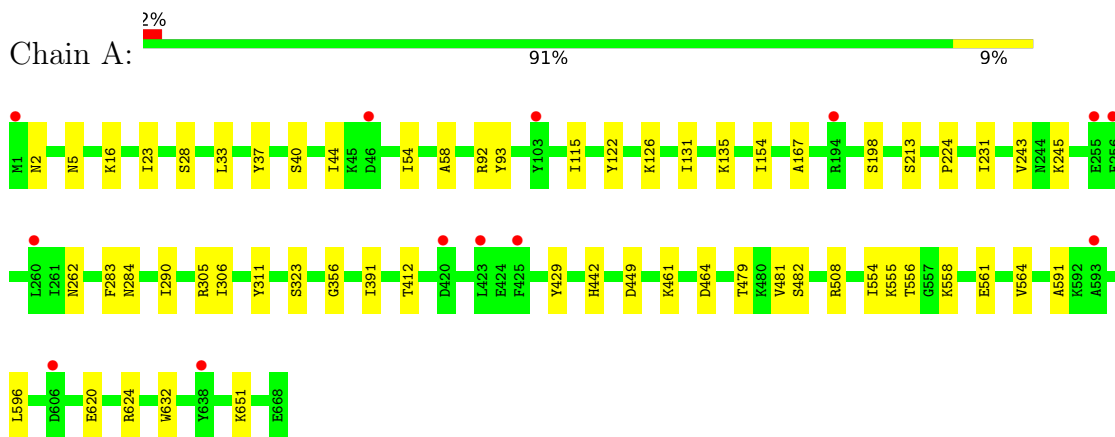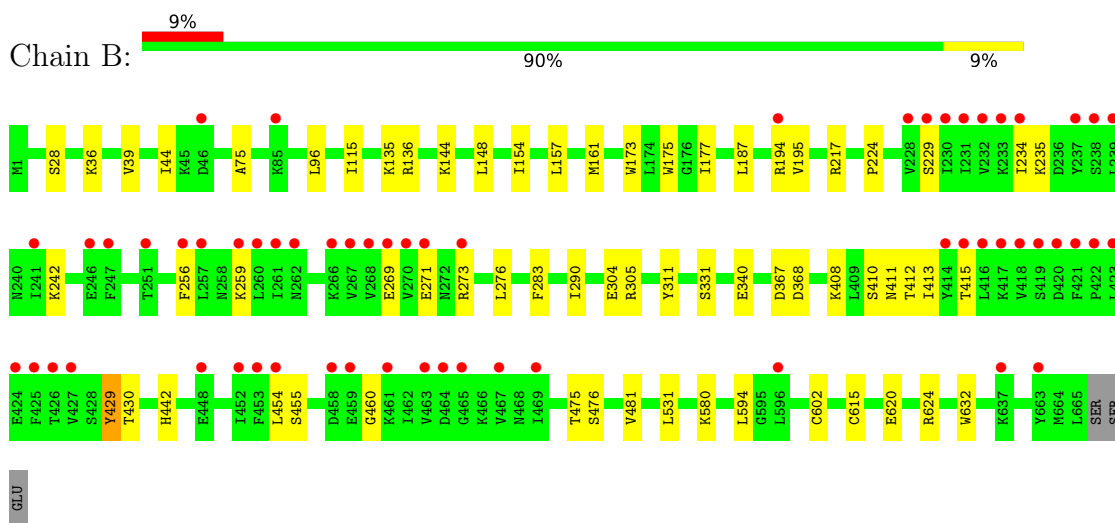
• Molecule 1: topoisomerase III

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	110.67Å 90.04Å 156.18Å 90.00° 100.52° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 48.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.10) 97.6 (48.73-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2747: ???)	Depositor
R, R_{free}	0.203 , 0.247 0.203 , 0.247	Depositor DCC
R_{free} test set	8485 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.1	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	0.95	EDS
Total number of atoms	22583	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8871e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.43	0/5506	0.58	0/7419
1	B	0.42	0/5485	0.57	0/7391
1	C	0.37	0/5497	0.53	0/7407
1	D	0.40	0/5491	0.54	1/7399 (0.0%)
All	All	0.40	0/21979	0.55	1/29616 (0.0%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	471	LEU	CA-CB-CG	6.30	129.80	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	283	PHE	Peptide
1	C	283	PHE	Peptide
1	D	283	PHE	Peptide

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	5401	0	5634	32	0
1	B	5380	0	5618	44	0
1	C	5392	0	5628	40	0
1	D	5386	0	5623	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	323	0	0	2	0
3	B	344	0	0	5	0
3	C	171	0	0	1	0
3	D	182	0	0	2	0
All	All	22583	0	22503	143	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 3.

All (143) 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:C:33:LEU:HD11	1:C:40:SER:HB3	1.68	0.75
1:A:231:ILE:HD13	1:A:464:ASP:HB3	1.75	0.68
1:B:217:ARG:NH2	1:B:475:THR:O	2.27	0.65
1:B:235:LYS:HD2	1:B:454:LEU:HD12	1.79	0.64
1:D:229:SER:HB3	1:D:242:LYS:HD3	1.78	0.64
1:A:135:LYS:HB3	1:A:154:ILE:HG23	1.82	0.62
1:D:167:ALA:HB2	1:D:561:GLU:HG3	1.82	0.61
1:B:580:LYS:NZ	3:B:902:HOH:O	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ILE:HD11	1:C:555:LYS:HE2	1.82	0.60
1:C:167:ALA:HB2	1:C:561:GLU:HG3	1.85	0.59
1:D:290:ILE:HD11	1:D:485:LYS:HD3	1.83	0.58
1:C:21:LYS:NZ	1:C:25:GLU:OE2	2.36	0.58
1:C:221:ILE:HG12	1:C:657:VAL:HG11	1.85	0.58
1:C:327:PRO:HD2	1:C:372:PRO:HB3	1.84	0.58
1:D:266:LYS:HB3	1:D:459:GLU:HG2	1.86	0.57
1:B:229:SER:HB3	1:B:242:LYS:HD3	1.87	0.56
1:B:175:TRP:HB3	3:B:1195:HOH:O	2.06	0.56
1:B:290:ILE:HG12	1:B:481:VAL:HG13	1.89	0.55
1:C:198:SER:OG	1:C:508:ARG:HD3	2.06	0.55
1:A:290:ILE:HG12	1:A:481:VAL:HG13	1.87	0.55
1:C:187:LEU:HD11	1:C:590:LEU:HB3	1.88	0.55
1:B:235:LYS:HZ2	1:B:455:SER:H	1.55	0.54
1:D:602:CYS:HB2	1:D:615:CYS:HB3	1.89	0.54
1:A:429:TYR:HB2	1:A:449:ASP:HB2	1.89	0.54
1:D:409:LEU:HD23	1:D:430:THR:HG21	1.89	0.54
1:B:256:PHE:HA	1:B:259:LYS:HE2	1.89	0.54
1:C:277:LEU:HB3	1:C:407:ALA:HB3	1.88	0.54
1:D:173:TRP:CE2	1:D:177:ILE:HG13	2.42	0.54
1:B:234:ILE:HB	1:B:460:GLY:HA3	1.90	0.54
1:C:599:ILE:HD12	1:C:608:GLU:HB2	1.89	0.53
1:B:367:ASP:OD1	1:B:368:ASP:N	2.39	0.53
1:A:591:ALA:HA	1:A:596:LEU:HD12	1.91	0.53
1:D:259:LYS:HB3	1:D:421:PHE:HE2	1.74	0.52
1:D:265:VAL:HG12	1:D:418:VAL:HG22	1.91	0.52
1:B:28:SER:HB3	1:B:44:ILE:HD12	1.91	0.52
1:B:187:LEU:HD23	1:B:195:VAL:HG12	1.89	0.52
1:B:412:THR:HB	1:B:429:TYR:CE2	2.44	0.52
1:D:217:ARG:NH1	1:D:475:THR:O	2.41	0.52
1:D:290:ILE:HG12	1:D:481:VAL:HG13	1.92	0.52
1:C:429:TYR:HB2	1:C:449:ASP:HB2	1.91	0.52
1:C:602:CYS:HB2	1:C:615:CYS:HB3	1.91	0.51
1:B:115:ILE:HG12	1:B:161:MET:HG3	1.92	0.51
1:B:136:ARG:HB2	1:B:157:LEU:HD23	1.92	0.51
1:A:305:ARG:NH1	3:A:919:HOH:O	2.44	0.51
1:C:271:GLU:HG2	1:C:273:ARG:HG2	1.93	0.50
1:C:84:ASP:HB3	1:C:87:SER:HB2	1.94	0.49
1:C:99:SER:HA	1:C:102:LYS:HE2	1.94	0.49
1:D:266:LYS:CB	1:D:459:GLU:HG2	2.42	0.49
1:C:46:ASP:OD1	1:C:46:ASP:N	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LEU:HD13	1:C:195:VAL:HG11	1.95	0.49
1:D:341:ASN:HB2	3:D:969:HOH:O	2.13	0.49
1:B:273:ARG:N	1:B:411:ASN:O	2.40	0.48
1:D:234:ILE:HB	1:D:460:GLY:HA3	1.94	0.48
1:C:474:PRO:HD3	1:C:652:SER:HB3	1.96	0.48
1:A:224:PRO:HD3	1:A:632:TRP:CE2	2.48	0.48
1:C:241:ILE:HD13	1:C:425:PHE:CE1	2.48	0.48
1:D:84:ASP:HB3	1:D:87:SER:HB2	1.94	0.48
1:B:269:GLU:HB3	1:B:415:THR:HB	1.95	0.48
1:B:194:ARG:HA	3:B:999:HOH:O	2.14	0.47
1:B:276:LEU:HD23	1:B:408:LYS:HG3	1.96	0.47
1:B:273:ARG:HB2	1:B:411:ASN:HB3	1.95	0.47
1:B:304:GLU:OE1	1:B:305:ARG:HD2	2.15	0.47
1:C:220:PHE:CG	1:C:474:PRO:HB3	2.49	0.47
1:B:144:LYS:NZ	3:B:921:HOH:O	2.47	0.47
1:D:262:ASN:HA	1:D:461:LYS:HE2	1.97	0.47
1:B:410:SER:O	1:B:430:THR:HA	2.15	0.46
1:A:284:ASN:HB3	1:A:323:SER:O	2.15	0.46
1:B:271:GLU:O	1:B:412:THR:HA	2.16	0.46
1:C:574:LYS:O	1:C:578:GLU:HG3	2.16	0.46
1:A:412:THR:HB	1:A:429:TYR:CE1	2.50	0.46
1:B:135:LYS:HB3	1:B:154:ILE:HG23	1.97	0.46
1:B:224:PRO:HD3	1:B:632:TRP:CE2	2.50	0.46
1:B:195:VAL:HG11	1:B:594:LEU:HD11	1.97	0.46
1:C:361:VAL:HG22	1:C:403:VAL:HG12	1.97	0.46
1:A:115:ILE:HD11	1:A:555:LYS:HE3	1.98	0.46
1:A:198:SER:OG	1:A:508:ARG:HD3	2.15	0.46
1:B:235:LYS:NZ	1:B:455:SER:H	2.14	0.46
1:B:411:ASN:HD21	1:B:413:ILE:HD11	1.80	0.46
1:A:122:TYR:OH	1:A:126:LYS:HD2	2.16	0.46
1:A:167:ALA:HB2	1:A:561:GLU:CG	2.46	0.45
1:B:194:ARG:NH1	3:B:928:HOH:O	2.49	0.45
1:C:352:ARG:HG2	1:C:359:TYR:OH	2.16	0.45
1:A:2:ASN:HB2	1:A:5:ASN:HB2	1.99	0.45
1:A:554:ILE:HD11	1:A:564:VAL:HG21	1.97	0.45
1:C:603:LYS:HG3	1:C:613:GLY:O	2.16	0.45
1:D:35:ARG:NH1	1:D:40:SER:OG	2.50	0.45
1:D:417:LYS:NZ	3:D:912:HOH:O	2.48	0.45
1:A:306:ILE:HG21	1:A:391:ILE:HG13	1.98	0.45
1:B:331:SER:HA	1:C:353:LYS:HE3	1.99	0.45
1:D:620:GLU:O	1:D:624:ARG:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.87	0.44
1:C:203:GLN:HG3	3:C:1045:HOH:O	2.17	0.44
1:D:327:PRO:HG2	1:D:330:ILE:HG12	1.99	0.44
1:C:349:ASP:O	1:C:353:LYS:HG2	2.18	0.44
1:A:37:TYR:O	1:A:92:ARG:HD2	2.18	0.44
1:A:556:THR:OG1	1:A:558:LYS:HG2	2.17	0.44
1:C:340:GLU:HB2	1:C:352:ARG:HH22	1.83	0.43
1:D:173:TRP:CE3	1:D:174:LEU:HD12	2.53	0.43
1:A:651:LYS:NZ	3:A:928:HOH:O	2.50	0.43
1:B:217:ARG:NH2	1:B:476:SER:HA	2.32	0.43
1:A:262:ASN:O	1:A:461:LYS:HE3	2.18	0.43
1:C:173:TRP:HE3	1:C:174:LEU:HD12	1.82	0.43
1:B:75:ALA:HB2	1:B:173:TRP:CZ3	2.53	0.43
1:A:620:GLU:O	1:A:624:ARG:HG2	2.18	0.43
1:B:28:SER:HB2	1:B:44:ILE:HG23	2.01	0.43
1:D:280:PRO:HD3	1:D:437:TRP:CE3	2.54	0.42
1:A:16:LYS:HA	1:A:16:LYS:HE2	1.99	0.42
1:A:33:LEU:HD11	1:A:40:SER:HB3	2.02	0.42
1:B:408:LYS:HE3	1:B:408:LYS:HB2	1.79	0.42
1:D:638:TYR:HB3	1:D:642:LYS:HD3	2.00	0.42
1:B:217:ARG:HH22	1:B:476:SER:HA	1.85	0.42
1:C:39:VAL:HB	1:C:96:LEU:HD22	2.01	0.42
1:C:421:PHE:CG	1:C:422:PRO:HD2	2.54	0.42
1:D:602:CYS:SG	1:D:603:LYS:N	2.93	0.42
1:B:36:LYS:HB3	1:B:96:LEU:HD13	2.01	0.42
1:C:543:MET:HE3	1:C:571:LYS:HE3	2.01	0.42
1:A:28:SER:HB3	1:A:44:ILE:HD12	2.02	0.42
1:A:243:VAL:HG12	1:A:245:LYS:H	1.84	0.42
1:A:131:ILE:HD12	1:A:131:ILE:HA	1.86	0.41
1:A:356:GLY:HA3	1:B:157:LEU:O	2.20	0.41
1:B:602:CYS:HB2	1:B:615:CYS:HB3	2.01	0.41
1:C:222:PRO:HB2	1:C:471:LEU:HB3	2.01	0.41
1:C:351:VAL:HG22	1:C:440:ILE:CD1	2.51	0.41
1:C:417:LYS:NZ	1:C:421:PHE:O	2.48	0.41
1:C:648:SER:HB2	1:C:661:VAL:HG11	2.02	0.41
1:A:479:THR:H	1:A:482:SER:HB3	1.86	0.41
1:D:270:VAL:HG13	1:D:414:TYR:CE1	2.56	0.41
1:D:332:ILE:HG21	1:D:359:TYR:HB3	2.03	0.41
1:A:122:TYR:CZ	1:A:126:LYS:HD2	2.56	0.41
1:D:21:LYS:HE2	1:D:25:GLU:OE2	2.21	0.41
1:B:620:GLU:O	1:B:624:ARG:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:PRO:HD3	1:C:632:TRP:NE1	2.36	0.41
1:C:651:LYS:HA	1:C:658:LYS:NZ	2.36	0.41
1:A:167:ALA:HB2	1:A:561:GLU:HG2	2.02	0.41
1:A:58:ALA:HB2	1:A:93:TYR:CE2	2.56	0.40
1:A:23:ILE:HG22	1:A:54:ILE:HD13	2.02	0.40
1:C:362:LYS:HA	1:C:362:LYS:HD2	1.91	0.40
1:B:173:TRP:CE2	1:B:177:ILE:HG13	2.57	0.40
1:C:491:ASN:O	1:C:548:GLU:HG3	2.22	0.40
1:D:256:PHE:HZ	1:D:423:LEU:HD12	1.87	0.40
1:D:341:ASN:O	1:D:345:ARG:NH2	2.54	0.40
1:B:39:VAL:HB	1:B:96:LEU:HD22	2.02	0.40
1:B:531:LEU:HD23	1:B:531:LEU:HA	1.91	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	666/668 (100%)	653 (98%)	13 (2%)	0	100	100
1	B	663/668 (99%)	649 (98%)	14 (2%)	0	100	100
1	C	665/668 (100%)	648 (97%)	17 (3%)	0	100	100
1	D	664/668 (99%)	649 (98%)	15 (2%)	0	100	100
All	All	2658/2672 (100%)	2599 (98%)	59 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	601/601 (100%)	598 (100%)	3 (0%)	88	92
1	B	598/601 (100%)	594 (99%)	4 (1%)	84	88
1	C	600/601 (100%)	596 (99%)	4 (1%)	84	88
1	D	599/601 (100%)	592 (99%)	7 (1%)	71	77
All	All	2398/2404 (100%)	2380 (99%)	18 (1%)	81	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	SER
1	A	311	TYR
1	A	442	HIS
1	B	311	TYR
1	B	340	GLU
1	B	429	TYR
1	B	442	HIS
1	C	213	SER
1	C	275	ARG
1	C	328	SER
1	C	442	HIS
1	D	155	SER
1	D	311	TYR
1	D	328	SER
1	D	367	ASP
1	D	442	HIS
1	D	471	LEU
1	D	602	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	212	ASN
1	C	532	ASN
1	D	188	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	668/668 (100%)	0.23	13 (1%)	66	71	17, 37, 66, 86	0
1	B	665/668 (99%)	0.50	59 (8%)	9	12	17, 36, 92, 135	0
1	C	667/668 (99%)	0.57	53 (7%)	12	16	21, 52, 76, 92	0
1	D	666/668 (99%)	0.55	61 (9%)	9	11	21, 48, 75, 92	0
All	All	2666/2672 (99%)	0.46	186 (6%)	16	20	17, 44, 78, 135	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	LEU	12.5
1	B	422	PRO	9.8
1	B	421	PHE	8.5
1	B	239	LEU	7.9
1	B	228	VAL	7.5
1	C	420	ASP	6.9
1	D	452	ILE	6.4
1	B	232	VAL	6.4
1	B	454	LEU	6.3
1	C	614	LEU	6.2
1	B	230	ILE	6.1
1	D	423	LEU	5.8
1	B	416	LEU	5.4
1	B	419	SER	5.2
1	B	467	VAL	5.2
1	B	266	LYS	5.1
1	B	418	VAL	4.9
1	D	576	ILE	4.9
1	B	231	ILE	4.7
1	B	425	PHE	4.7
1	C	4	CYS	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	417	LYS	4.5
1	D	580	LYS	4.5
1	C	228	VAL	4.5
1	D	610	TYR	4.3
1	D	425	PHE	4.3
1	D	418	VAL	4.2
1	D	647	ILE	4.2
1	C	467	VAL	4.2
1	B	453	PHE	4.2
1	D	416	LEU	4.1
1	C	638	TYR	4.0
1	B	262	ASN	4.0
1	D	46	ASP	4.0
1	A	606	ASP	3.9
1	C	665	LEU	3.9
1	B	251	THR	3.9
1	D	1	MET	3.8
1	B	424	GLU	3.8
1	C	32	ILE	3.8
1	C	70	PHE	3.8
1	B	237	TYR	3.8
1	D	626	LEU	3.7
1	C	67	GLU	3.7
1	B	414	TYR	3.7
1	C	72	VAL	3.7
1	C	41	TYR	3.6
1	B	260	LEU	3.6
1	C	422	PRO	3.6
1	B	420	ASP	3.6
1	C	247	PHE	3.5
1	B	234	ILE	3.5
1	C	246	GLU	3.4
1	D	453	PHE	3.4
1	C	183	LEU	3.4
1	C	613	GLY	3.4
1	D	656	TYR	3.3
1	A	194	ARG	3.3
1	D	275	ARG	3.2
1	C	103	TYR	3.2
1	B	459	GLU	3.2
1	C	194	ARG	3.2
1	D	270	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	429	TYR	3.2
1	D	477	ARG	3.2
1	D	413	ILE	3.2
1	B	458	ASP	3.1
1	B	256	PHE	3.1
1	D	526	TYR	3.1
1	C	525	PHE	3.1
1	A	425	PHE	3.0
1	C	1	MET	3.0
1	D	600	VAL	3.0
1	C	657	VAL	3.0
1	D	72	VAL	2.9
1	B	259	LYS	2.9
1	C	48	ASN	2.9
1	D	47	HIS	2.9
1	D	215	ILE	2.9
1	D	248	GLU	2.9
1	D	523	LEU	2.9
1	D	417	LYS	2.9
1	B	415	THR	2.9
1	B	267	VAL	2.8
1	D	467	VAL	2.8
1	A	260	LEU	2.8
1	B	464	ASP	2.8
1	C	421	PHE	2.8
1	C	42	TRP	2.7
1	A	256	PHE	2.7
1	B	247	PHE	2.7
1	D	448	GLU	2.7
1	C	649	SER	2.7
1	B	461	LYS	2.7
1	C	217	ARG	2.7
1	B	465	GLY	2.6
1	B	463	VAL	2.6
1	C	88	TYR	2.6
1	B	271	GLU	2.6
1	D	596	LEU	2.6
1	D	451	PRO	2.6
1	C	190	PHE	2.6
1	B	261	ILE	2.6
1	B	233	LYS	2.6
1	C	612	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	420	ASP	2.6
1	D	619	TYR	2.6
1	A	420	ASP	2.5
1	C	7	ASN	2.5
1	B	46	ASP	2.5
1	D	421	PHE	2.5
1	B	273	ARG	2.5
1	B	238	SER	2.5
1	D	49	SER	2.5
1	A	423	LEU	2.4
1	B	637	LYS	2.4
1	C	610	TYR	2.4
1	B	426	THR	2.4
1	B	596	LEU	2.4
1	C	255	GLU	2.4
1	D	427	VAL	2.4
1	D	422	PRO	2.4
1	B	229	SER	2.4
1	D	607	LEU	2.4
1	B	427	VAL	2.4
1	B	452	ILE	2.4
1	A	46	ASP	2.4
1	A	638	TYR	2.4
1	B	663	TYR	2.4
1	C	226	PHE	2.3
1	D	274	VAL	2.3
1	D	629	VAL	2.3
1	D	219	LEU	2.3
1	C	174	LEU	2.3
1	C	661	VAL	2.3
1	C	651	LYS	2.3
1	D	273	ARG	2.3
1	C	47	HIS	2.3
1	D	645	LYS	2.3
1	D	616	LYS	2.3
1	C	667	SER	2.3
1	C	34	CYS	2.2
1	C	43	ILE	2.2
1	C	37	TYR	2.2
1	C	66	GLY	2.2
1	C	179	VAL	2.2
1	C	564	VAL	2.2

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	267	VAL	2.2
1	B	269	GLU	2.2
1	B	85	LYS	2.2
1	B	270	VAL	2.2
1	D	450	LYS	2.2
1	D	414	TYR	2.2
1	C	266	LYS	2.2
1	D	609	GLN	2.1
1	C	239	LEU	2.1
1	D	3	LEU	2.1
1	D	468	ASN	2.1
1	D	534	PHE	2.1
1	D	663	TYR	2.1
1	C	653	THR	2.1
1	B	241	ILE	2.1
1	D	454	LEU	2.1
1	D	612	ASP	2.1
1	C	621	ALA	2.1
1	D	660	ILE	2.1
1	A	103	TYR	2.1
1	A	593	ALA	2.1
1	D	640	HIS	2.1
1	C	83	ILE	2.1
1	A	255	GLU	2.1
1	C	664	MET	2.1
1	B	268	VAL	2.1
1	B	246	GLU	2.0
1	B	448	GLU	2.0
1	B	194	ARG	2.0
1	B	469	ILE	2.0
1	D	194	ARG	2.0
1	A	1	MET	2.0
1	D	581	VAL	2.0
1	C	451	PRO	2.0
1	B	257	LEU	2.0
1	C	662	THR	2.0
1	D	633	LYS	2.0
1	D	276	LEU	2.0
1	D	527	ILE	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 monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	ZN	A	801	1/1	0.98	0.07	52,52,52,52	0
2	ZN	B	801	1/1	0.99	0.04	38,38,38,38	0
2	ZN	C	801	1/1	0.99	0.03	60,60,60,60	0
2	ZN	D	801	1/1	0.99	0.04	54,54,54,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.