



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:36 AM UTC

PDB ID : 6K8N / pdb_00006k8n
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)

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

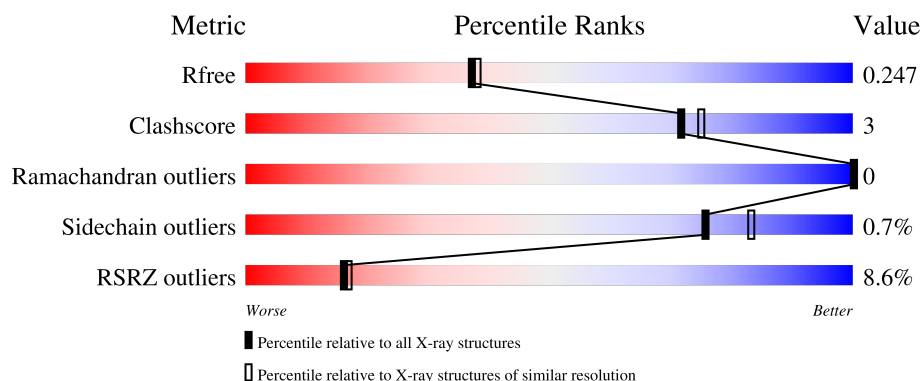
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	668	3% 91% 9%
1	B	668	9% 90% 9%
1	C	668	11% 88% 11%
1	D	668	11% 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	C	N	O	S	0	0	0
			5401	3498	908	980	15			
1	B	665	Total	C	N	O	S	0	0	0
			5380	3487	905	973	15			
1	C	667	Total	C	N	O	S	0	0	0
			5392	3493	907	977	15			
1	D	666	Total	C	N	O	S	0	0	0
			5386	3490	906	975	15			

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 (CCD ID: ZN) (formula: Zn).

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

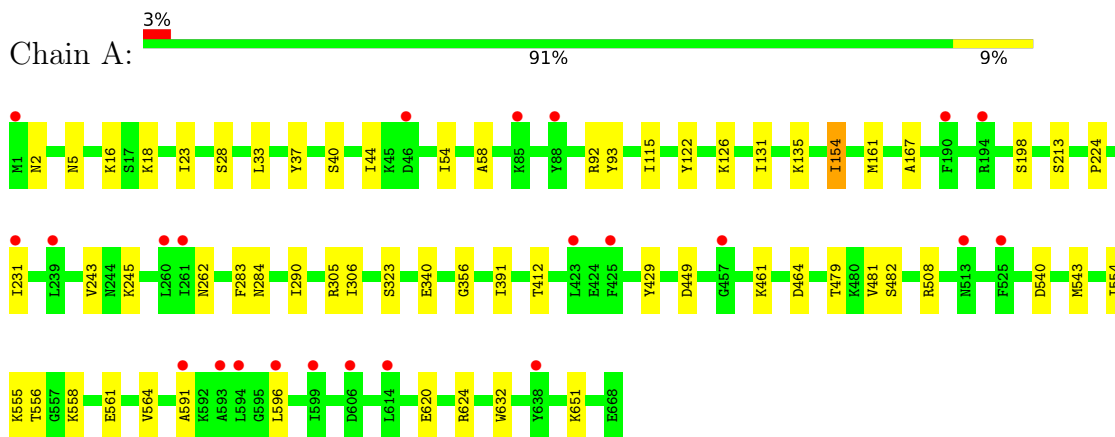
- Molecule 3 is water.

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

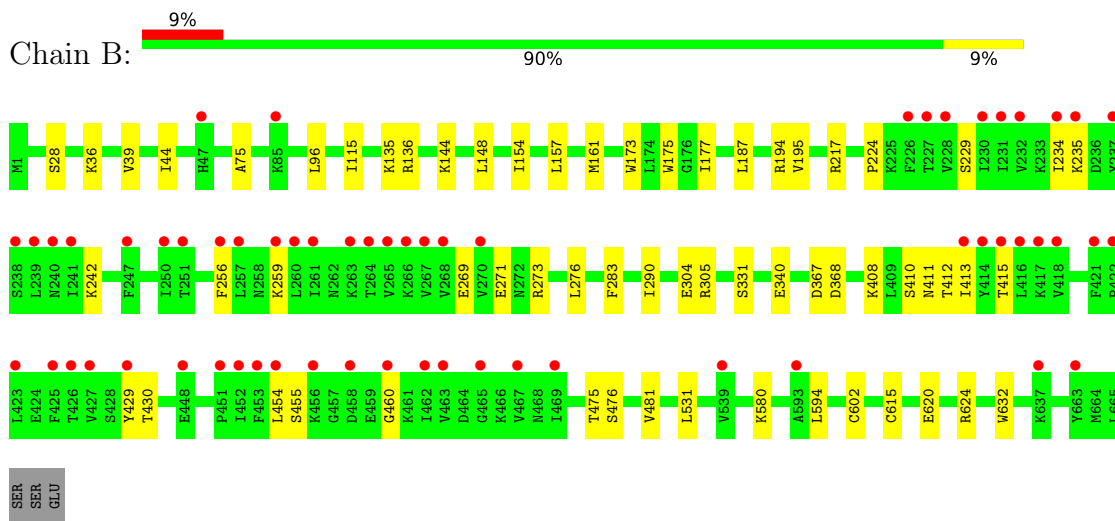
3 Residue-property plots [i](#)

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.

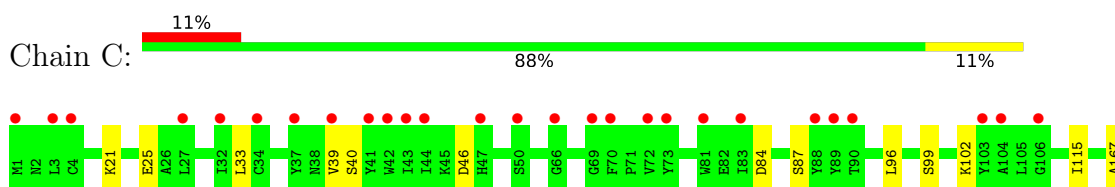
• Molecule 1: topoisomerase III

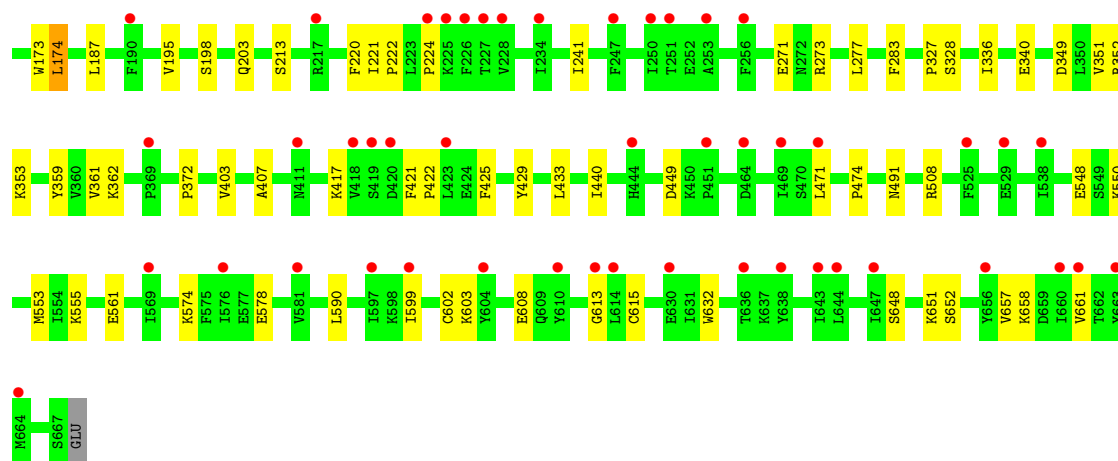


• Molecule 1: topoisomerase III

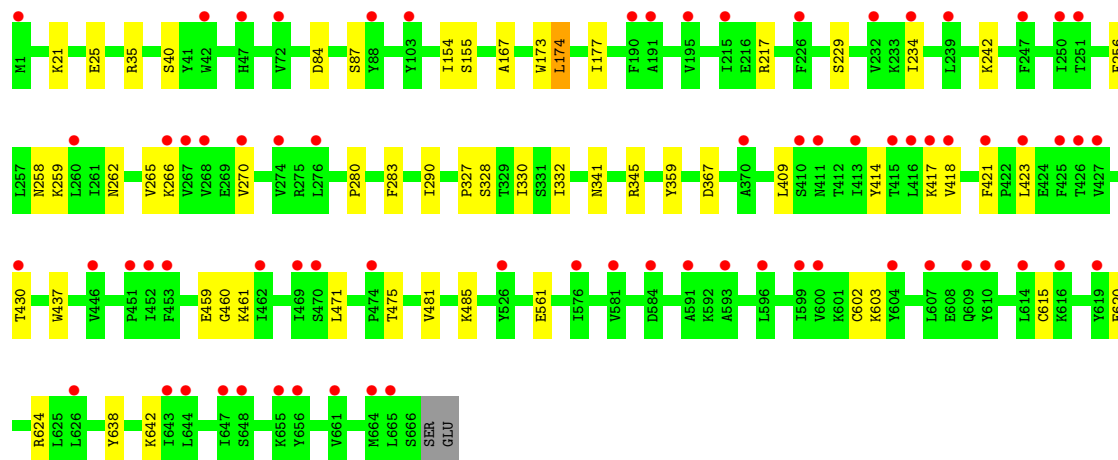


• Molecule 1: topoisomerase III





- 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 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.10) 97.6 (50.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.82%)	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)	0.33 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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

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	0.38	0/5506	0.55	0/7419
1	B	0.38	0/5485	0.55	0/7391
1	C	0.31	0/5497	0.50	0/7407
1	D	0.35	0/5491	0.50	0/7399
All	All	0.36	0/21979	0.53	0/29616

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.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	PHE	Peptide
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	35	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	3	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	146	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 (146) 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
1:C:115:ILE:HD11	1:C:555:LYS:HE2	1.82	0.60
1:A:18:LYS:NZ	3:A:905:HOH:O	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:550:LYS:HA	1:C:553:MET:HE3	1.89	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:417:LYS:NZ	1:C:421:PHE:O	2.48	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
1:A:540:ASP:CB	1:A:543:MET:HE3	2.47	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:161:MET:HE2	1:A:161:MET:HB2	1.98	0.40
1:A:651:LYS:NZ	3:A:928:HOH:O	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/601 (100%)	598 (100%)	3 (0%)	81	88
1	B	598/601 (100%)	597 (100%)	1 (0%)	87	93
1	C	600/601 (100%)	595 (99%)	5 (1%)	73	81
1	D	599/601 (100%)	592 (99%)	7 (1%)	63	72
All	All	2398/2404 (100%)	2382 (99%)	16 (1%)	76	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ILE
1	A	213	SER
1	A	340	GLU
1	B	340	GLU
1	C	174	LEU
1	C	213	SER
1	C	328	SER
1	C	336	ILE
1	C	433	LEU
1	D	154	ILE
1	D	155	SER
1	D	174	LEU
1	D	258	ASN
1	D	328	SER
1	D	367	ASP
1	D	471	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	ASN
1	B	7	ASN
1	B	8	ASN
1	B	95	GLN
1	B	258	ASN
1	B	322	ASN
1	B	411	ASN
1	C	212	ASN
1	C	262	ASN
1	C	532	ASN
1	D	5	ASN

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Mol	Chain	Res	Type
1	D	127	ASN
1	D	153	ASN
1	D	188	GLN
1	D	371	HIS
1	D	468	ASN

5.3.3 RNA [i](#)

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](#)

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 [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	668/668 (100%)	0.27	23 (3%)	48 50	17, 37, 66, 86	0
1	B	665/668 (99%)	0.45	60 (9%)	15 16	17, 36, 92, 135	0
1	C	667/668 (99%)	0.79	74 (11%)	10 10	21, 52, 76, 92	0
1	D	666/668 (99%)	0.69	72 (10%)	11 11	21, 48, 75, 92	0
All	All	2666/2672 (99%)	0.55	229 (8%)	16 17	17, 44, 78, 135	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	LEU	6.6
1	B	234	ILE	6.2
1	B	421	PHE	5.4
1	B	418	VAL	5.3
1	B	232	VAL	5.3
1	B	267	VAL	5.3
1	D	418	VAL	5.0
1	B	261	ILE	4.9
1	B	416	LEU	4.9
1	D	423	LEU	4.8
1	B	453	PHE	4.8
1	B	228	VAL	4.7
1	C	420	ASP	4.4
1	B	460	GLY	4.4
1	D	453	PHE	4.3
1	B	423	LEU	4.3
1	D	195	VAL	4.2
1	B	454	LEU	4.2
1	C	614	LEU	4.2
1	B	231	ILE	4.1
1	B	265	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	225	LYS	4.1
1	B	230	ILE	4.0
1	C	369	PRO	3.9
1	C	250	ILE	3.8
1	D	416	LEU	3.8
1	B	257	LEU	3.8
1	B	462	ILE	3.8
1	C	643	ILE	3.7
1	D	274	VAL	3.6
1	D	413	ILE	3.6
1	C	42	TRP	3.6
1	C	41	TYR	3.6
1	D	610	TYR	3.6
1	B	427	VAL	3.5
1	D	425	PHE	3.5
1	C	88	TYR	3.5
1	B	240	ASN	3.5
1	B	260	LEU	3.5
1	C	569	ILE	3.4
1	B	235	LYS	3.4
1	C	599	ILE	3.4
1	B	268	VAL	3.2
1	D	656	TYR	3.2
1	D	276	LEU	3.2
1	B	422	PRO	3.2
1	A	594	LEU	3.1
1	A	425	PHE	3.1
1	B	85	LYS	3.1
1	B	463	VAL	3.1
1	B	241	ILE	3.1
1	B	452	ILE	3.1
1	A	260	LEU	3.0
1	C	226	PHE	3.0
1	C	4	CYS	3.0
1	C	34	CYS	3.0
1	D	665	LEU	3.0
1	B	467	VAL	2.9
1	D	270	VAL	2.9
1	A	1	MET	2.9
1	A	638	TYR	2.9
1	D	47	HIS	2.9
1	B	425	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	606	ASP	2.9
1	D	234	ILE	2.9
1	D	451	PRO	2.9
1	D	417	LYS	2.9
1	D	526	TYR	2.9
1	C	66	GLY	2.9
1	B	266	LYS	2.8
1	D	619	TYR	2.8
1	C	471	LEU	2.8
1	D	72	VAL	2.8
1	C	228	VAL	2.8
1	D	600	VAL	2.8
1	D	88	TYR	2.8
1	D	191	ALA	2.8
1	D	607	LEU	2.8
1	B	426	THR	2.8
1	C	72	VAL	2.8
1	D	427	VAL	2.8
1	C	597	ILE	2.8
1	B	458	ASP	2.7
1	D	226	PHE	2.7
1	C	663	TYR	2.7
1	C	217	ARG	2.7
1	B	469	ILE	2.7
1	A	457	GLY	2.7
1	C	3	LEU	2.7
1	D	267	VAL	2.7
1	C	43	ILE	2.7
1	B	637	LYS	2.7
1	C	247	PHE	2.7
1	D	626	LEU	2.7
1	C	451	PRO	2.7
1	C	604	TYR	2.7
1	B	413	ILE	2.7
1	C	576	ILE	2.7
1	D	247	PHE	2.6
1	C	638	TYR	2.6
1	C	630	GLU	2.6
1	A	423	LEU	2.6
1	C	423	LEU	2.6
1	D	268	VAL	2.6
1	C	529	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	596	LEU	2.6
1	B	256	PHE	2.6
1	D	661	VAL	2.6
1	B	264	THR	2.6
1	A	190	PHE	2.5
1	C	525	PHE	2.5
1	C	647	ILE	2.5
1	D	250	ILE	2.5
1	D	462	ILE	2.5
1	C	89	TYR	2.5
1	A	591	ALA	2.5
1	C	90	THR	2.5
1	B	250	ILE	2.5
1	C	613	GLY	2.5
1	D	446	VAL	2.5
1	B	238	SER	2.5
1	B	414	TYR	2.5
1	D	1	MET	2.5
1	B	226	PHE	2.5
1	C	227	THR	2.4
1	B	593	ALA	2.4
1	B	263	LYS	2.4
1	C	81	TRP	2.4
1	C	418	VAL	2.4
1	B	251	THR	2.4
1	D	415	THR	2.4
1	D	426	THR	2.4
1	A	513	ASN	2.4
1	D	411	ASN	2.4
1	D	609	GLN	2.4
1	B	270	VAL	2.4
1	C	661	VAL	2.4
1	D	643	ILE	2.4
1	A	88	TYR	2.4
1	D	604	TYR	2.4
1	C	27	LEU	2.4
1	C	190	PHE	2.4
1	C	32	ILE	2.4
1	C	469	ILE	2.4
1	D	215	ILE	2.4
1	C	610	TYR	2.3
1	A	593	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	644	LEU	2.3
1	B	247	PHE	2.3
1	D	469	ILE	2.3
1	B	415	THR	2.3
1	B	448	GLU	2.3
1	B	429	TYR	2.3
1	A	596	LEU	2.3
1	C	70	PHE	2.3
1	B	47	HIS	2.3
1	B	539	VAL	2.3
1	C	581	VAL	2.3
1	B	451	PRO	2.3
1	D	593	ALA	2.3
1	B	465	GLY	2.3
1	C	37	TYR	2.3
1	C	69	GLY	2.3
1	C	656	TYR	2.3
1	D	239	LEU	2.3
1	D	614	LEU	2.3
1	D	232	VAL	2.3
1	D	103	TYR	2.3
1	D	576	ILE	2.2
1	D	251	THR	2.2
1	D	430	THR	2.2
1	D	616	LYS	2.2
1	C	103	TYR	2.2
1	D	42	TRP	2.2
1	C	224	PRO	2.2
1	D	266	LYS	2.2
1	C	1	MET	2.2
1	B	227	THR	2.2
1	C	44	ILE	2.2
1	C	251	THR	2.2
1	D	452	ILE	2.2
1	D	474	PRO	2.2
1	D	664	MET	2.2
1	C	253	ALA	2.2
1	D	190	PHE	2.1
1	D	599	ILE	2.1
1	C	47	HIS	2.1
1	D	260	LEU	2.1
1	C	50	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	410	SER	2.1
1	A	85	LYS	2.1
1	B	456	LYS	2.1
1	C	234	ILE	2.1
1	C	660	ILE	2.1
1	D	581	VAL	2.1
1	A	194	ARG	2.1
1	D	644	LEU	2.1
1	C	411	ASN	2.1
1	A	46	ASP	2.1
1	A	261	ILE	2.1
1	A	599	ILE	2.1
1	C	83	ILE	2.1
1	C	538	ILE	2.1
1	D	647	ILE	2.1
1	D	421	PHE	2.1
1	A	239	LEU	2.1
1	A	614	LEU	2.1
1	C	419	SER	2.1
1	C	464	ASP	2.1
1	B	237	TYR	2.1
1	A	231	ILE	2.1
1	C	39	VAL	2.1
1	C	256	PHE	2.1
1	D	470	SER	2.1
1	C	664	MET	2.0
1	D	584	ASP	2.0
1	C	444	HIS	2.0
1	C	636	THR	2.0
1	B	259	LYS	2.0
1	B	417	LYS	2.0
1	D	655	LYS	2.0
1	A	525	PHE	2.0
1	D	648	SER	2.0
1	C	104	ALA	2.0
1	D	370	ALA	2.0
1	D	591	ALA	2.0
1	C	106	GLY	2.0
1	B	663	TYR	2.0
1	C	73	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	ZN	D	801	1/1	0.98	0.08	54,54,54,54	0
2	ZN	B	801	1/1	0.99	0.08	38,38,38,38	0
2	ZN	C	801	1/1	0.99	0.09	60,60,60,60	0
2	ZN	A	801	1/1	0.99	0.04	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.