



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 PM UTC

PDB ID : 5TUA / pdb_00005tua
Title : structure of a Na⁺-selective mutant of two-pore channel from Arabidopsis thaliana AtTPC1
Authors : Guo, J.; Zeng, W.; Jiang, Y.
Deposited on : 2016-11-05
Resolution : 3.30 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

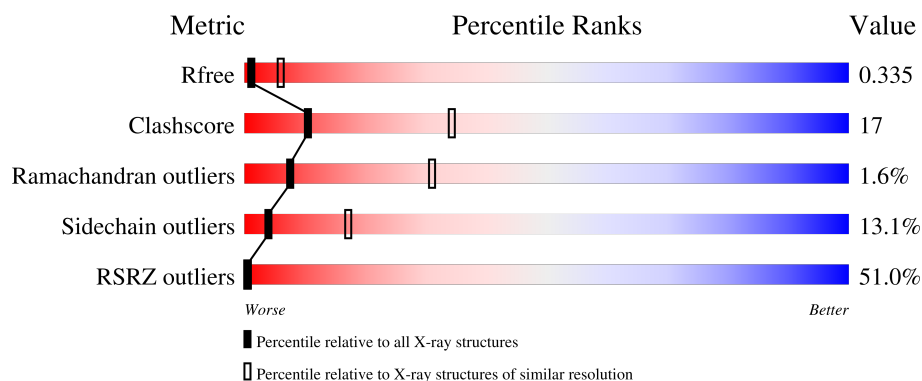
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	739	43% 47% 32% 6% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5126 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 Two pore calcium channel protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	627	Total	C	N	O	S	0	0	0
			5114	3399	787	907	21			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ALA	SER	conflict	UNP Q94KI8
A	629	VAL	MET	conflict	UNP Q94KI8
A	630	ASN	GLY	conflict	UNP Q94KI8
A	734	SER	-	expression tag	UNP Q94KI8
A	735	THR	-	expression tag	UNP Q94KI8
A	736	ALA	-	expression tag	UNP Q94KI8
A	737	GLY	-	expression tag	UNP Q94KI8
A	738	LEU	-	expression tag	UNP Q94KI8
A	739	VAL	-	expression tag	UNP Q94KI8

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is BARIUM ION (CCD ID: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	Ba	0	0
			9	9		

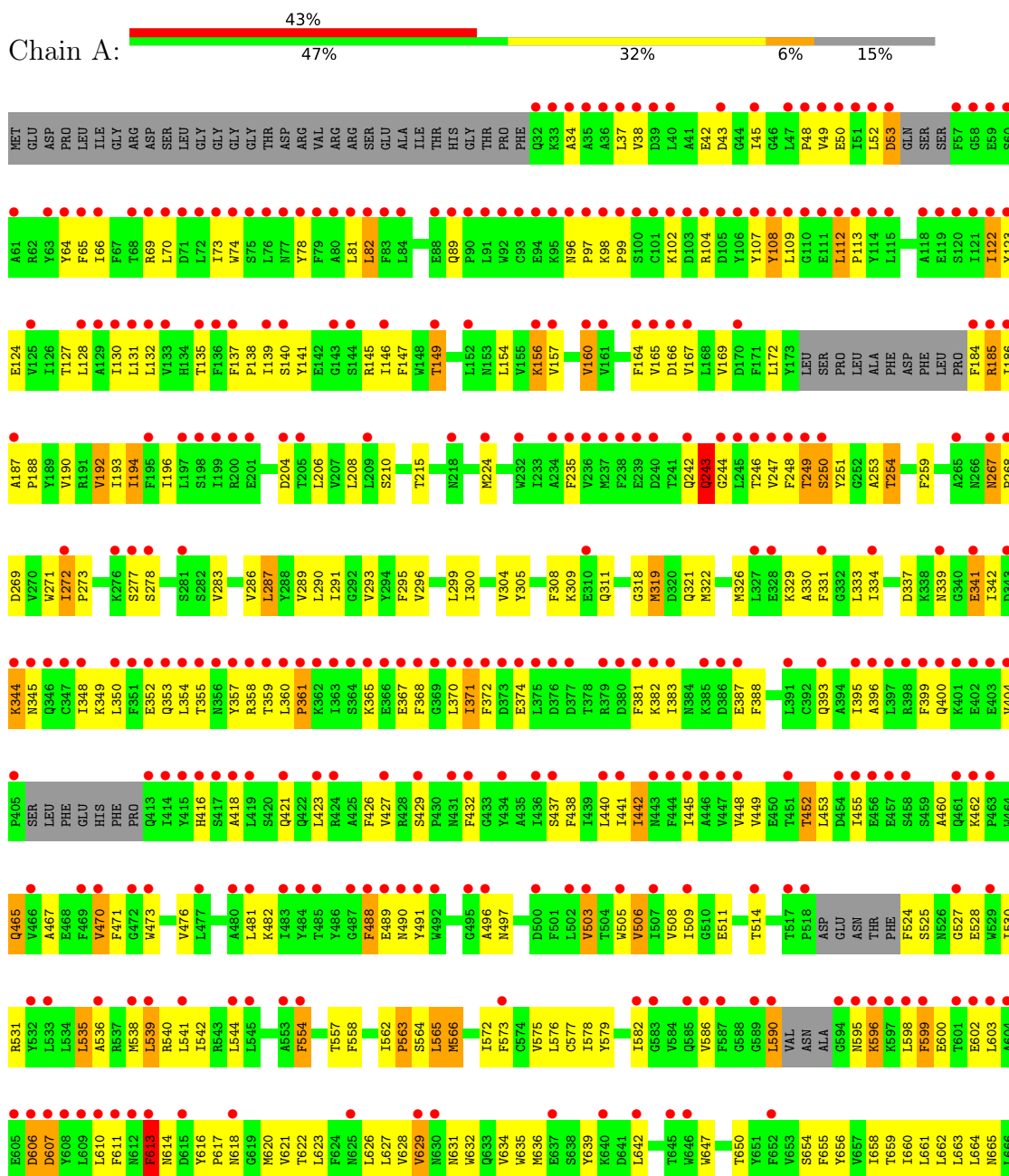
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

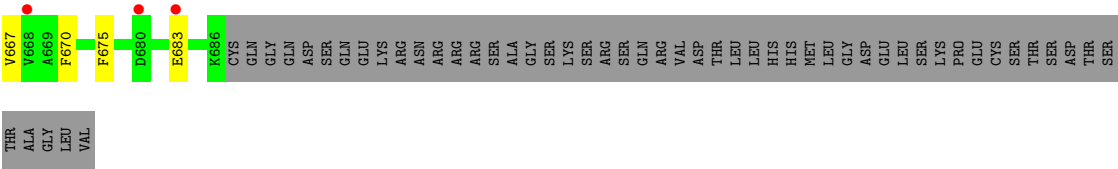
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0

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: Two pore calcium channel protein 1





THR
ALA
GLY
LEU
VAL

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.53Å 156.37Å 217.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.59 – 3.30 44.59 – 3.30	Depositor EDS
% Data completeness (in resolution range)	62.8 (44.59-3.30) 63.2 (44.59-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.65 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.310 , 0.323 0.313 , 0.335	Depositor DCC
R_{free} test set	727 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.045 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	5126	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BA, NA, CA

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	0.26	0/5241	0.51	2/7128 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	565	LEU	CA-C-N	5.00	126.34	120.09
1	A	565	LEU	C-N-CA	5.00	126.34	120.09

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	5114	0	5091	173	0
2	A	2	0	0	0	0
3	A	9	0	0	0	0
4	A	1	0	0	0	0
All	All	5126	0	5091	173	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 17.

All (173) 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:A:250:SER:OG	1:A:251:TYR:N	2.11	0.79
1:A:536:ALA:O	1:A:539:LEU:HB2	1.83	0.78
1:A:572:ILE:HD11	1:A:627:LEU:HD11	1.66	0.76
1:A:577:CYS:HA	1:A:620:MET:HE1	1.66	0.76
1:A:66:ILE:HD13	1:A:140:SER:HB2	1.68	0.74
1:A:603:LEU:HD13	1:A:606:ASP:HB2	1.68	0.73
1:A:613:PHE:H	1:A:618:ASN:HB3	1.53	0.73
1:A:367:GLU:HA	1:A:370:LEU:HB2	1.71	0.71
1:A:348:ILE:O	1:A:352:GLU:HB2	1.90	0.71
1:A:112:LEU:HD22	1:A:113:PRO:HD2	1.73	0.71
1:A:353:GLN:O	1:A:357:TYR:HB2	1.91	0.71
1:A:124:GLU:O	1:A:128:LEU:HB2	1.91	0.70
1:A:190:VAL:O	1:A:194:ILE:HB	1.92	0.70
1:A:595:ASN:O	1:A:599:PHE:HB2	1.92	0.69
1:A:145:ARG:O	1:A:149:THR:HB	1.94	0.68
1:A:38:VAL:HG21	1:A:353:GLN:HB2	1.74	0.67
1:A:367:GLU:O	1:A:371:ILE:HB	1.94	0.66
1:A:656:TYR:O	1:A:660:ILE:HB	1.95	0.66
1:A:370:LEU:O	1:A:374:GLU:HB3	1.95	0.66
1:A:344:LYS:NZ	1:A:345:ASN:OD1	2.29	0.65
1:A:74:TRP:O	1:A:78:TYR:CB	2.46	0.64
1:A:43:ASP:HB3	1:A:326:MET:HE1	1.78	0.63
1:A:607:ASP:HA	1:A:610:LEU:HB3	1.81	0.62
1:A:37:LEU:CD1	1:A:334:ILE:HB	2.31	0.60
1:A:535:LEU:HB2	1:A:538:MET:HE2	1.83	0.60
1:A:259:PHE:HE2	1:A:632:TRP:HH2	1.47	0.60
1:A:354:LEU:HD11	1:A:395:ILE:HG21	1.82	0.60
1:A:235:PHE:HB2	1:A:254:THR:HG21	1.84	0.60
1:A:438:PHE:HA	1:A:441:ILE:HD12	1.84	0.60
1:A:81:LEU:HD11	1:A:127:THR:HA	1.83	0.59
1:A:53:ASP:OD1	1:A:53:ASP:N	2.35	0.59
1:A:157:VAL:HA	1:A:160:VAL:HB	1.83	0.59
1:A:350:LEU:HD21	1:A:388:PHE:CE1	2.36	0.59
1:A:249:THR:HB	1:A:253:ALA:HB2	1.84	0.59
1:A:334:ILE:HD11	1:A:349:LYS:HZ2	1.67	0.59
1:A:337:ASP:OD2	1:A:339:ASN:ND2	2.35	0.58
1:A:623:LEU:HD23	1:A:626:LEU:HD12	1.84	0.58
1:A:291:ILE:O	1:A:295:PHE:HB2	2.04	0.58
1:A:524:PHE:O	1:A:528:GLU:N	2.33	0.58
1:A:655:PHE:O	1:A:659:THR:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:VAL:HA	1:A:473:TRP:HD1	1.68	0.57
1:A:286:VAL:O	1:A:290:LEU:HB2	2.04	0.57
1:A:598:LEU:O	1:A:602:GLU:CB	2.53	0.57
1:A:342:ILE:O	1:A:382:LYS:HA	2.05	0.55
1:A:448:VAL:O	1:A:452:THR:HB	2.06	0.55
1:A:331:PHE:HB2	1:A:388:PHE:CD2	2.41	0.55
1:A:511:GLU:HA	1:A:531:ARG:NH1	2.21	0.55
1:A:404:VAL:HA	1:A:490:ASN:HD21	1.71	0.55
1:A:505:TRP:HA	1:A:508:VAL:HG22	1.89	0.54
1:A:563:PRO:O	1:A:566:MET:HB2	2.08	0.54
1:A:579:TYR:HA	1:A:582:ILE:HD12	1.88	0.54
1:A:43:ASP:O	1:A:48:PRO:HD2	2.08	0.54
1:A:488:PHE:HD1	1:A:489:GLU:HG2	1.72	0.54
1:A:122:ILE:HG13	1:A:123:TYR:N	2.21	0.54
1:A:606:ASP:OD1	1:A:606:ASP:N	2.35	0.54
1:A:370:LEU:O	1:A:374:GLU:CB	2.56	0.53
1:A:138:PRO:HA	1:A:141:TYR:CE2	2.43	0.53
1:A:139:ILE:HG12	1:A:147:PHE:CG	2.43	0.53
1:A:107:TYR:OH	1:A:596:LYS:HG2	2.09	0.53
1:A:300:ILE:O	1:A:304:VAL:HG23	2.08	0.53
1:A:426:PHE:O	1:A:429:SER:OG	2.27	0.53
1:A:449:VAL:O	1:A:452:THR:HG22	2.08	0.53
1:A:49:VAL:HG22	1:A:322:MET:HE2	1.91	0.52
1:A:109:LEU:HD22	1:A:611:PHE:HB2	1.91	0.52
1:A:45:ILE:HG12	1:A:396:ALA:HB2	1.92	0.52
1:A:34:ALA:HB3	1:A:353:GLN:HE22	1.75	0.52
1:A:208:LEU:HD21	1:A:308:PHE:HD1	1.74	0.52
1:A:165:VAL:O	1:A:169:VAL:HG23	2.10	0.52
1:A:112:LEU:HG	1:A:617:PRO:HG2	1.92	0.52
1:A:272:ILE:HG22	1:A:273:PRO:HD3	1.90	0.51
1:A:329:LYS:O	1:A:333:LEU:HG	2.10	0.51
1:A:554:PHE:N	1:A:554:PHE:HD1	2.07	0.51
1:A:539:LEU:HD23	1:A:542:ILE:HD13	1.92	0.51
1:A:138:PRO:HG2	1:A:147:PHE:HE2	1.75	0.51
1:A:267:ASN:O	1:A:271:TRP:NE1	2.43	0.51
1:A:166:ASP:OD2	1:A:187:ALA:HB2	2.11	0.50
1:A:437:SER:O	1:A:440:LEU:HG	2.11	0.50
1:A:554:PHE:N	1:A:554:PHE:CD1	2.76	0.50
1:A:393:GLN:HA	1:A:396:ALA:HB3	1.92	0.50
1:A:131:LEU:O	1:A:135:THR:HG23	2.11	0.50
1:A:453:LEU:HD13	1:A:460:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PHE:O	1:A:167:VAL:HG12	2.12	0.50
1:A:330:ALA:O	1:A:333:LEU:N	2.43	0.49
1:A:467:ALA:O	1:A:470:VAL:HG12	2.11	0.49
1:A:664:LEU:HA	1:A:667:VAL:HG22	1.94	0.49
1:A:452:THR:HA	1:A:455:ILE:HG12	1.94	0.49
1:A:89:GLN:HG3	1:A:188:PRO:HB3	1.95	0.49
1:A:42:GLU:HB2	1:A:358:ARG:HG3	1.93	0.49
1:A:344:LYS:HB2	1:A:381:PHE:CB	2.43	0.49
1:A:564:SER:HB2	1:A:670:PHE:HZ	1.77	0.49
1:A:558:PHE:O	1:A:562:ILE:HG13	2.12	0.49
1:A:359:THR:HG21	1:A:400:GLN:HA	1.94	0.49
1:A:70:LEU:HB2	1:A:137:PHE:CE1	2.48	0.48
1:A:395:ILE:O	1:A:400:GLN:HB2	2.13	0.48
1:A:527:GLY:HA2	1:A:530:ILE:HG22	1.95	0.48
1:A:208:LEU:HD21	1:A:308:PHE:CD1	2.48	0.48
1:A:573:PHE:O	1:A:576:LEU:HB2	2.14	0.48
1:A:81:LEU:HD13	1:A:130:ILE:HD12	1.96	0.48
1:A:596:LYS:O	1:A:600:GLU:HG2	2.14	0.48
1:A:503:VAL:O	1:A:506:VAL:HG12	2.14	0.48
1:A:96:ASN:CG	1:A:97:PRO:HD3	2.38	0.48
1:A:438:PHE:O	1:A:442:ILE:HG22	2.14	0.48
1:A:602:GLU:O	1:A:603:LEU:HD23	2.13	0.48
1:A:322:MET:HE1	1:A:326:MET:HG3	1.95	0.47
1:A:622:THR:OG1	1:A:635:TRP:NE1	2.47	0.47
1:A:250:SER:O	1:A:254:THR:HB	2.14	0.47
1:A:470:VAL:HA	1:A:473:TRP:CD1	2.47	0.47
1:A:590:LEU:HD22	1:A:642:LEU:HD22	1.95	0.47
1:A:337:ASP:OD1	1:A:337:ASP:N	2.35	0.47
1:A:187:ALA:HB3	1:A:188:PRO:HD3	1.97	0.47
1:A:135:THR:HG22	1:A:156:LYS:HE2	1.97	0.47
1:A:65:PHE:O	1:A:69:ARG:HG3	2.15	0.46
1:A:37:LEU:HG	1:A:330:ALA:HB1	1.97	0.46
1:A:268:PRO:HG2	1:A:269:ASP:OD1	2.15	0.46
1:A:383:ILE:HD11	1:A:387:GLU:HG3	1.97	0.46
1:A:462:LYS:HA	1:A:465:GLN:HB3	1.96	0.46
1:A:496:ALA:HB1	1:A:540:ARG:HD2	1.98	0.46
1:A:243:GLN:NE2	1:A:271:TRP:HA	2.30	0.46
1:A:289:VAL:O	1:A:293:VAL:HB	2.15	0.46
1:A:506:VAL:HA	1:A:509:ILE:HG22	1.98	0.46
1:A:576:LEU:HD22	1:A:623:LEU:HB3	1.97	0.46
1:A:616:TYR:CE2	1:A:620:MET:HE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HG23	1:A:396:ALA:HB1	1.98	0.45
1:A:481:LEU:HD12	1:A:482:LYS:N	2.30	0.45
1:A:248:PHE:C	1:A:250:SER:H	2.25	0.45
1:A:613:PHE:HB3	1:A:639:TYR:OH	2.17	0.45
1:A:334:ILE:HD12	1:A:350:LEU:HD22	1.99	0.44
1:A:650:THR:O	1:A:654:SER:HB3	2.16	0.44
1:A:112:LEU:HD22	1:A:113:PRO:CD	2.46	0.44
1:A:242:GLN:C	1:A:244:GLY:H	2.24	0.44
1:A:355:THR:HA	1:A:361:PRO:HD2	1.99	0.44
1:A:78:TYR:O	1:A:82:LEU:HG	2.16	0.44
1:A:49:VAL:HA	1:A:322:MET:HE2	2.00	0.44
1:A:575:VAL:HG21	1:A:663:LEU:HD11	1.98	0.44
1:A:631:ASN:O	1:A:634:VAL:HG22	2.18	0.44
1:A:650:THR:O	1:A:654:SER:CB	2.66	0.44
1:A:319:MET:HE2	1:A:319:MET:HB2	1.66	0.44
1:A:247:VAL:HG13	1:A:254:THR:HB	2.00	0.43
1:A:603:LEU:HD22	1:A:606:ASP:CG	2.42	0.43
1:A:66:ILE:O	1:A:69:ARG:HB2	2.18	0.43
1:A:146:ILE:O	1:A:149:THR:HG22	2.18	0.43
1:A:554:PHE:HD1	1:A:554:PHE:H	1.67	0.43
1:A:296:VAL:O	1:A:300:ILE:HG13	2.18	0.43
1:A:661:LEU:O	1:A:665:ASN:ND2	2.36	0.43
1:A:70:LEU:O	1:A:74:TRP:HB3	2.19	0.42
1:A:361:PRO:HA	1:A:399:PHE:CD1	2.53	0.42
1:A:473:TRP:O	1:A:476:VAL:HG12	2.18	0.42
1:A:109:LEU:HD22	1:A:611:PHE:HD2	1.84	0.42
1:A:445:ILE:O	1:A:448:VAL:HG22	2.19	0.42
1:A:193:ILE:O	1:A:196:ILE:HG12	2.18	0.42
1:A:138:PRO:HG2	1:A:147:PHE:CE2	2.54	0.42
1:A:365:LYS:H	1:A:368:PHE:HB2	1.85	0.42
1:A:305:TYR:HE1	1:A:309:LYS:HE2	1.84	0.42
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.91	0.42
1:A:283:VAL:O	1:A:287:LEU:HB2	2.19	0.42
1:A:491:TYR:CE1	1:A:497:ASN:HB3	2.55	0.42
1:A:453:LEU:HD23	1:A:453:LEU:HA	1.92	0.42
1:A:38:VAL:HG11	1:A:353:GLN:O	2.19	0.41
1:A:37:LEU:HD13	1:A:334:ILE:HB	1.99	0.41
1:A:557:THR:HG21	1:A:675:PHE:HB2	2.02	0.41
1:A:530:ILE:HG23	1:A:531:ARG:HG2	2.03	0.41
1:A:107:TYR:HH	1:A:596:LYS:HG2	1.84	0.41
1:A:242:GLN:O	1:A:244:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLU:HA	1:A:383:ILE:O	2.20	0.41
1:A:318:GLY:O	1:A:321:GLN:HB2	2.21	0.41
1:A:130:ILE:H	1:A:130:ILE:HG13	1.68	0.41
1:A:432:PHE:CZ	1:A:481:LEU:HD11	2.56	0.41
1:A:184:PHE:CD1	1:A:185:ARG:HG2	2.56	0.40
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.94	0.40
1:A:541:LEU:O	1:A:544:LEU:HB3	2.20	0.40
1:A:658:ILE:O	1:A:662:LEU:HB3	2.22	0.40
1:A:192:VAL:HG21	1:A:578:ILE:HG13	2.03	0.40
1:A:416:HIS:C	1:A:418:ALA:H	2.28	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	615/739 (83%)	561 (91%)	44 (7%)	10 (2%)	7	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	TYR
1	A	361	PRO
1	A	629	VAL
1	A	249	THR
1	A	613	PHE
1	A	104	ARG
1	A	243	GLN
1	A	563	PRO
1	A	647	TRP
1	A	99	PRO

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	551/660 (84%)	479 (87%)	72 (13%)	4 17

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	53	ASP
1	A	64	TYR
1	A	73	ILE
1	A	82	LEU
1	A	98	LYS
1	A	102	LYS
1	A	108	TYR
1	A	112	LEU
1	A	122	ILE
1	A	132	LEU
1	A	149	THR
1	A	154	LEU
1	A	156	LYS
1	A	160	VAL
1	A	185	ARG
1	A	186	ILE
1	A	192	VAL
1	A	194	ILE
1	A	204	ASP
1	A	206	LEU
1	A	210	SER
1	A	215	THR
1	A	224	MET
1	A	243	GLN
1	A	246	THR
1	A	250	SER
1	A	254	THR
1	A	267	ASN
1	A	272	ILE

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Mol	Chain	Res	Type
1	A	277	SER
1	A	278	SER
1	A	287	LEU
1	A	299	LEU
1	A	311	GLN
1	A	319	MET
1	A	341	GLU
1	A	344	LYS
1	A	360	LEU
1	A	371	ILE
1	A	372	PHE
1	A	421	GLN
1	A	423	LEU
1	A	427	VAL
1	A	442	ILE
1	A	452	THR
1	A	465	GLN
1	A	470	VAL
1	A	471	PHE
1	A	488	PHE
1	A	503	VAL
1	A	506	VAL
1	A	514	THR
1	A	525	SER
1	A	535	LEU
1	A	539	LEU
1	A	554	PHE
1	A	565	LEU
1	A	566	MET
1	A	586	VAL
1	A	590	LEU
1	A	596	LYS
1	A	599	PHE
1	A	606	ASP
1	A	607	ASP
1	A	613	PHE
1	A	614	ASN
1	A	621	VAL
1	A	628	VAL
1	A	629	VAL
1	A	636	MET
1	A	683	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	311	GLN
1	A	547	ASN
1	A	614	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 12 ligands modelled in this entry, 12 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	627/739 (84%)	2.30	320 (51%) 0 0	16, 67, 114, 162	0

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	LEU	8.6
1	A	356	ASN	8.5
1	A	184	PHE	7.9
1	A	248	PHE	7.4
1	A	69	ARG	7.3
1	A	399	PHE	7.3
1	A	112	LEU	6.7
1	A	49	VAL	6.6
1	A	357	TYR	6.5
1	A	683	GLU	6.3
1	A	250	SER	6.2
1	A	489	GLU	6.1
1	A	39	ASP	6.1
1	A	529	TRP	6.0
1	A	380	ASP	6.0
1	A	366	GLU	6.0
1	A	60	SER	5.9
1	A	200	ARG	5.8
1	A	105	ASP	5.7
1	A	170	ASP	5.7
1	A	95	LYS	5.5
1	A	103	ASP	5.5
1	A	419	LEU	5.4
1	A	123	TYR	5.4
1	A	533	LEU	5.4
1	A	345	ASN	5.4
1	A	371	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	347	CYS	5.4
1	A	400	GLN	5.4
1	A	97	PRO	5.3
1	A	440	LEU	5.3
1	A	32	GLN	5.3
1	A	113	PRO	5.2
1	A	370	LEU	5.2
1	A	373	ASP	5.2
1	A	90	PRO	5.2
1	A	68	THR	5.2
1	A	437	SER	5.2
1	A	488	PHE	5.1
1	A	74	TRP	5.1
1	A	277	SER	5.0
1	A	609	LEU	4.9
1	A	218	ASN	4.9
1	A	204	ASP	4.9
1	A	354	LEU	4.8
1	A	91	LEU	4.7
1	A	107	TYR	4.7
1	A	414	ILE	4.6
1	A	607	ASP	4.6
1	A	104	ARG	4.6
1	A	680	ASP	4.5
1	A	198	SER	4.5
1	A	608	TYR	4.5
1	A	135	THR	4.4
1	A	484	TYR	4.4
1	A	532	TYR	4.4
1	A	51	ILE	4.4
1	A	541	LEU	4.4
1	A	361	PRO	4.4
1	A	79	PHE	4.4
1	A	447	VAL	4.4
1	A	120	SER	4.4
1	A	396	ALA	4.3
1	A	89	GLN	4.3
1	A	348	ILE	4.2
1	A	595	ASN	4.2
1	A	106	TYR	4.2
1	A	50	GLU	4.2
1	A	93	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	610	LEU	4.1
1	A	334	ILE	4.1
1	A	239	GLU	4.1
1	A	235	PHE	4.1
1	A	346	GLN	4.1
1	A	359	THR	4.0
1	A	101	CYS	4.0
1	A	100	SER	4.0
1	A	166	ASP	4.0
1	A	364	SER	4.0
1	A	514	THR	4.0
1	A	38	VAL	4.0
1	A	99	PRO	4.0
1	A	53	ASP	4.0
1	A	72	LEU	4.0
1	A	65	PHE	3.9
1	A	268	PRO	3.9
1	A	143	GLY	3.9
1	A	47	LEU	3.9
1	A	457	GLU	3.9
1	A	199	ILE	3.9
1	A	57	PHE	3.9
1	A	372	PHE	3.9
1	A	387	GLU	3.9
1	A	431	ASN	3.9
1	A	596	LYS	3.8
1	A	381	PHE	3.8
1	A	343	ASP	3.8
1	A	601	THR	3.8
1	A	490	ASN	3.8
1	A	612	ASN	3.8
1	A	185	ARG	3.8
1	A	114	TYR	3.8
1	A	605	GLU	3.8
1	A	477	LEU	3.8
1	A	382	LYS	3.8
1	A	429	SER	3.8
1	A	353	GLN	3.7
1	A	244	GLY	3.7
1	A	386	ASP	3.7
1	A	111	GLU	3.7
1	A	102	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	35	ALA	3.7
1	A	434	TYR	3.7
1	A	156	LYS	3.7
1	A	405	PRO	3.7
1	A	108	TYR	3.7
1	A	149	THR	3.7
1	A	444	PHE	3.7
1	A	339	ASN	3.6
1	A	63	TYR	3.6
1	A	398	ARG	3.6
1	A	606	ASP	3.6
1	A	393	GLN	3.5
1	A	403	GLU	3.5
1	A	415	TYR	3.5
1	A	83	PHE	3.5
1	A	360	LEU	3.5
1	A	473	TRP	3.5
1	A	363	ILE	3.5
1	A	404	VAL	3.5
1	A	139	ILE	3.5
1	A	110	GLY	3.4
1	A	64	TYR	3.4
1	A	36	ALA	3.4
1	A	278	SER	3.4
1	A	34	ALA	3.4
1	A	395	ILE	3.4
1	A	247	VAL	3.4
1	A	487	GLY	3.4
1	A	401	LYS	3.3
1	A	598	LEU	3.3
1	A	242	GLN	3.3
1	A	59	GLU	3.3
1	A	368	PHE	3.3
1	A	81	LEU	3.2
1	A	365	LYS	3.2
1	A	350	LEU	3.2
1	A	417	SER	3.2
1	A	413	GLN	3.2
1	A	77	ASN	3.2
1	A	121	ILE	3.2
1	A	645	THR	3.1
1	A	518	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	237	MET	3.1
1	A	195	PHE	3.1
1	A	427	VAL	3.1
1	A	613	PHE	3.1
1	A	491	TYR	3.1
1	A	469	PHE	3.1
1	A	586	VAL	3.1
1	A	40	LEU	3.1
1	A	397	LEU	3.1
1	A	140	SER	3.0
1	A	146	ILE	3.0
1	A	500	ASP	3.0
1	A	76	LEU	3.0
1	A	423	LEU	3.0
1	A	52	LEU	3.0
1	A	88	GLU	3.0
1	A	82	LEU	3.0
1	A	144	SER	3.0
1	A	391	LEU	3.0
1	A	454	ASP	3.0
1	A	416	HIS	3.0
1	A	652	PHE	3.0
1	A	246	THR	3.0
1	A	341	GLU	2.9
1	A	492	TRP	2.9
1	A	483	ILE	2.9
1	A	61	ALA	2.9
1	A	75	SER	2.9
1	A	58	GLY	2.9
1	A	585	GLN	2.9
1	A	132	LEU	2.9
1	A	249	THR	2.9
1	A	369	GLY	2.9
1	A	73	ILE	2.9
1	A	131	LEU	2.9
1	A	603	LEU	2.9
1	A	48	PRO	2.9
1	A	451	THR	2.9
1	A	267	ASN	2.9
1	A	379	ARG	2.9
1	A	377	ASP	2.8
1	A	485	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	362	LYS	2.8
1	A	137	PHE	2.8
1	A	281	SER	2.8
1	A	98	LYS	2.8
1	A	583	GLY	2.8
1	A	625	ASN	2.8
1	A	418	ALA	2.8
1	A	461	GLN	2.8
1	A	536	ALA	2.8
1	A	165	VAL	2.8
1	A	544	LEU	2.8
1	A	481	LEU	2.7
1	A	130	ILE	2.7
1	A	238	PHE	2.7
1	A	436	ILE	2.7
1	A	590	LEU	2.7
1	A	310	GLU	2.7
1	A	470	VAL	2.7
1	A	463	PRO	2.7
1	A	495	GLY	2.7
1	A	234	ALA	2.7
1	A	96	ASN	2.7
1	A	376	ASP	2.7
1	A	70	LEU	2.6
1	A	327	LEU	2.6
1	A	480	ALA	2.6
1	A	66	ILE	2.6
1	A	587	PHE	2.6
1	A	466	VAL	2.6
1	A	33	LYS	2.6
1	A	441	ILE	2.6
1	A	351	PHE	2.6
1	A	502	LEU	2.6
1	A	118	ALA	2.6
1	A	496	ALA	2.6
1	A	43	ASP	2.6
1	A	119	GLU	2.6
1	A	133	VAL	2.6
1	A	344	LYS	2.6
1	A	597	LYS	2.6
1	A	573	PHE	2.5
1	A	445	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	331	PHE	2.5
1	A	245	LEU	2.5
1	A	629	VAL	2.5
1	A	355	THR	2.5
1	A	109	LEU	2.5
1	A	80	ALA	2.5
1	A	78	TYR	2.5
1	A	160	VAL	2.5
1	A	448	VAL	2.5
1	A	553	ALA	2.5
1	A	599	PHE	2.5
1	A	594	GLY	2.5
1	A	458	SER	2.4
1	A	402	GLU	2.4
1	A	538	MET	2.4
1	A	611	PHE	2.4
1	A	276	LYS	2.4
1	A	125	VAL	2.4
1	A	527	GLY	2.4
1	A	128	LEU	2.4
1	A	505	TRP	2.4
1	A	446	ALA	2.4
1	A	509	ILE	2.4
1	A	224	MET	2.4
1	A	201	GLU	2.3
1	A	187	ALA	2.3
1	A	604	ALA	2.3
1	A	618	ASN	2.3
1	A	71	ASP	2.3
1	A	152	LEU	2.3
1	A	554	PHE	2.3
1	A	352	GLU	2.3
1	A	92	TRP	2.3
1	A	646	TRP	2.3
1	A	265	ALA	2.3
1	A	129	ALA	2.3
1	A	539	LEU	2.3
1	A	630	ASN	2.3
1	A	94	GLU	2.3
1	A	197	LEU	2.2
1	A	161	VAL	2.2
1	A	236	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	503	VAL	2.2
1	A	375	LEU	2.2
1	A	472	GLY	2.2
1	A	164	PHE	2.2
1	A	517	THR	2.2
1	A	186	ILE	2.2
1	A	272	ILE	2.2
1	A	167	VAL	2.2
1	A	582	ILE	2.2
1	A	640	LYS	2.2
1	A	122	ILE	2.2
1	A	507	ILE	2.2
1	A	642	LEU	2.2
1	A	328	GLU	2.2
1	A	602	GLU	2.2
1	A	367	GLU	2.1
1	A	615	ASP	2.1
1	A	205	THR	2.1
1	A	209	LEU	2.1
1	A	424	ARG	2.1
1	A	443	ASN	2.1
1	A	84	LEU	2.1
1	A	358	ARG	2.1
1	A	374	GLU	2.1
1	A	157	VAL	2.1
1	A	240	ASP	2.1
1	A	421	GLN	2.1
1	A	383	ILE	2.1
1	A	455	ILE	2.1
1	A	432	PHE	2.1
1	A	545	LEU	2.0
1	A	232	TRP	2.0
1	A	589	GLY	2.0
1	A	385	LYS	2.0
1	A	462	LYS	2.0
1	A	637	GLU	2.0
1	A	668	VAL	2.0
1	A	45	ILE	2.0
1	A	136	PHE	2.0
1	A	456	GLU	2.0
1	A	115	LEU	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
3	BA	A	811	1/1	0.40	0.38	168,168,168,168	1
3	BA	A	809	1/1	0.71	0.26	180,180,180,180	0
3	BA	A	807	1/1	0.76	0.25	156,156,156,156	0
4	NA	A	812	1/1	0.85	0.21	27,27,27,27	1
2	CA	A	801	1/1	0.86	0.10	107,107,107,107	0
2	CA	A	802	1/1	0.89	0.10	79,79,79,79	0
3	BA	A	805	1/1	0.91	0.43	124,124,124,124	1
3	BA	A	808	1/1	0.92	0.14	136,136,136,136	0
3	BA	A	810	1/1	0.94	0.38	118,118,118,118	1
3	BA	A	804	1/1	0.95	0.05	87,87,87,87	0
3	BA	A	803	1/1	0.95	0.05	57,57,57,57	0
3	BA	A	806	1/1	0.96	0.04	108,108,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.