



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:54 AM UTC

PDB ID : 5IWR / pdb_00005iwr
Title : Structure of Transient Receptor Potential (TRP) channel TRPV6 in the presence of barium
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Deposited on : 2016-03-22
Resolution : 3.85 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

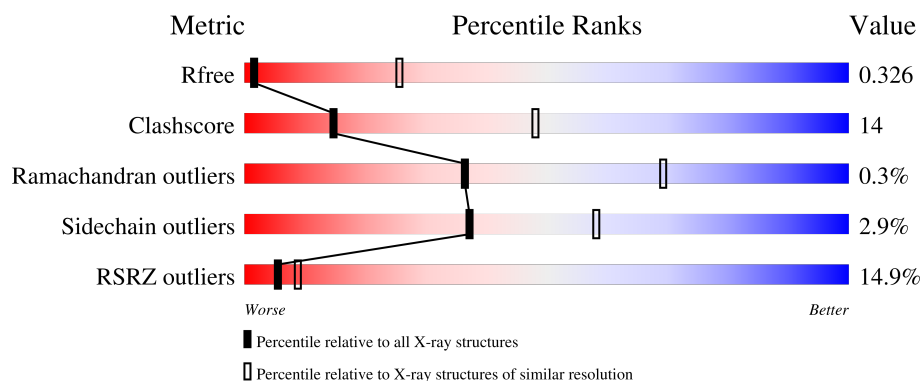
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

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	672	13% 61% 22% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4775 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 Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4756	3074	799	851	32			

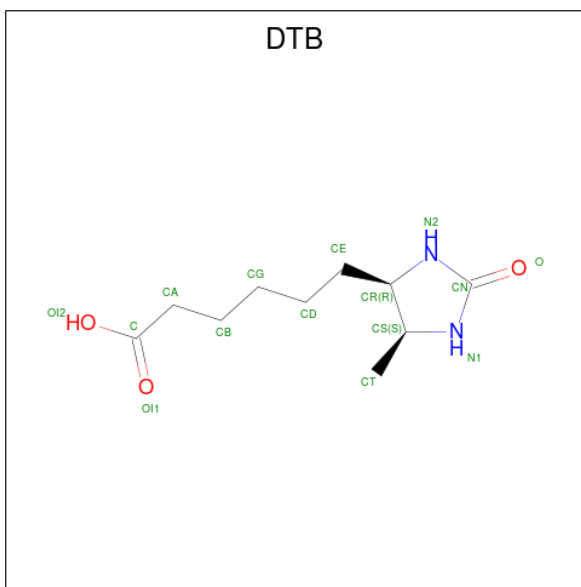
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	TYR	ILE	engineered mutation	UNP Q9R186
A	92	ASN	LEU	engineered mutation	UNP Q9R186
A	96	GLN	MET	engineered mutation	UNP Q9R186
A	495	GLN	LEU	engineered mutation	UNP Q9R186
A	670	VAL	-	expression tag	UNP Q9R186
A	671	PRO	-	expression tag	UNP Q9R186
A	672	ARG	-	expression tag	UNP Q9R186

- Molecule 2 is BARIUM ION (CCD ID: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ba	0	0
			4	4		

- Molecule 3 is 6-(5-METHYL-2-OXO-IMIDAZOLIDIN-4-YL)-HEXANOIC ACID (CCD ID: DTB) (formula: C₁₀H₁₈N₂O₃).

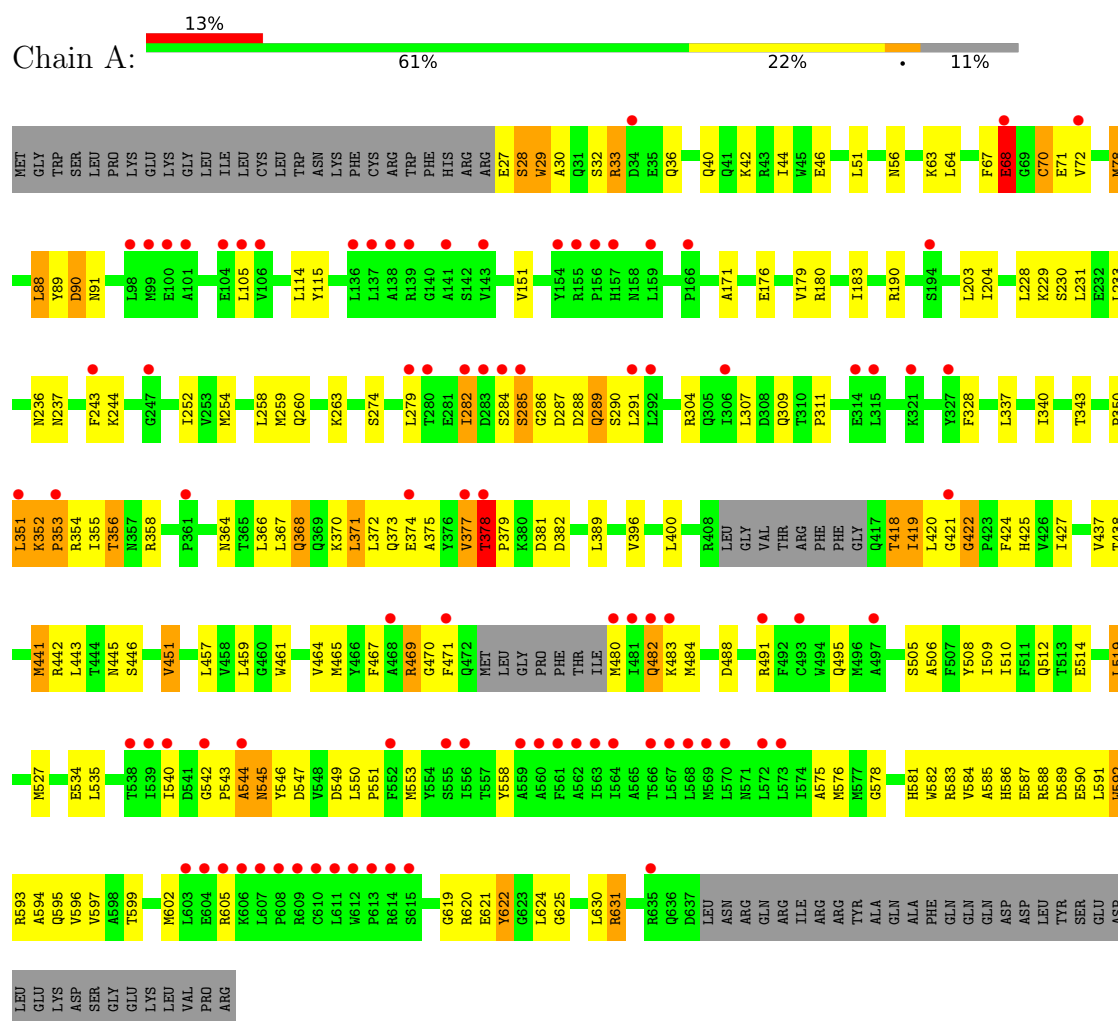


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	10	2	3	0	0

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: Transient receptor potential cation channel subfamily V member 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.35Å 144.35Å 113.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 3.85 49.56 – 3.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.56-3.85) 99.8 (49.56-3.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.283 , 0.323 0.297 , 0.326	Depositor DCC
R_{free} test set	593 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	154.4	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 75.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	4775	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

5.1 Standard geometry

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

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	0.37	4/4864 (0.1%)	1.05	53/6607 (0.8%)

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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	PRO	N-CD	8.89	1.60	1.47
1	A	68	GLU	C-N	-8.28	1.21	1.33
1	A	288	ASP	N-CA	-5.07	1.40	1.46
1	A	352	LYS	CA-C	-5.03	1.47	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	ASP	N-CA-C	-17.96	90.96	113.23
1	A	482	GLN	N-CA-C	16.97	129.87	111.03
1	A	29	TRP	N-CA-CB	-16.73	84.84	110.44
1	A	382	ASP	N-CA-C	-16.32	92.99	113.23
1	A	351	LEU	N-CA-C	16.03	141.21	107.70
1	A	351	LEU	CB-CA-C	-15.75	86.91	111.17
1	A	289	GLN	N-CA-C	15.07	134.17	113.37
1	A	68	GLU	N-CA-C	14.85	131.81	111.92
1	A	30	ALA	N-CA-C	-14.68	95.36	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	GLU	CA-C-N	13.36	147.59	121.41
1	A	68	GLU	C-N-CA	13.36	147.59	121.41
1	A	288	ASP	N-CA-C	-12.79	100.04	114.62
1	A	290	SER	N-CA-C	12.18	129.69	110.32
1	A	290	SER	N-CA-CB	-11.84	91.11	110.41
1	A	546	TYR	CB-CA-C	-10.90	91.95	110.81
1	A	377	VAL	N-CA-C	-10.21	93.50	108.71
1	A	70	CYS	N-CA-C	9.79	124.53	110.14
1	A	469	ARG	CB-CA-C	-8.78	92.94	110.42
1	A	70	CYS	N-CA-CB	-8.68	97.76	110.70
1	A	68	GLU	CB-CA-C	-7.73	101.11	111.63
1	A	28	SER	N-CA-C	-7.67	94.45	110.80
1	A	482	GLN	CB-CA-C	-7.48	99.36	110.95
1	A	418	THR	CA-C-N	-7.46	113.62	123.17
1	A	418	THR	C-N-CA	-7.46	113.62	123.17
1	A	576	MET	N-CA-C	7.35	120.22	111.33
1	A	422	GLY	N-CA-C	-7.32	97.41	112.34
1	A	68	GLU	O-C-N	-7.30	112.84	122.47
1	A	29	TRP	N-CA-C	7.03	121.88	113.16
1	A	605	ARG	N-CA-C	6.89	118.88	111.36
1	A	483	LYS	N-CA-C	-6.86	104.78	113.01
1	A	544	ALA	N-CA-C	6.69	121.82	112.93
1	A	285	SER	CA-C-N	6.60	127.30	119.98
1	A	285	SER	C-N-CA	6.60	127.30	119.98
1	A	575	ALA	CB-CA-C	6.57	121.13	110.95
1	A	64	LEU	N-CA-C	-6.55	105.91	114.04
1	A	284	SER	N-CA-C	6.53	119.14	110.53
1	A	419	ILE	N-CA-C	6.41	118.03	106.61
1	A	353	PRO	CA-N-CD	-6.37	103.08	112.00
1	A	63	LYS	CB-CA-C	-6.22	98.20	110.27
1	A	545	ASN	N-CA-C	6.22	118.79	111.02
1	A	356	THR	N-CA-C	6.17	119.41	110.28
1	A	575	ALA	N-CA-C	-5.80	104.60	111.03
1	A	90	ASP	N-CA-C	-5.78	98.49	110.80
1	A	378	THR	CA-C-N	-5.74	112.68	119.05
1	A	378	THR	C-N-CA	-5.74	112.68	119.05
1	A	451	VAL	CB-CA-C	-5.58	108.44	114.35
1	A	352	LYS	CA-C-N	-5.55	114.54	120.03
1	A	352	LYS	C-N-CA	-5.55	114.54	120.03
1	A	470	GLY	N-CA-C	-5.47	100.21	113.18
1	A	33	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	A	421	GLY	N-CA-C	-5.19	100.88	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	LEU	N-CA-C	5.13	116.68	111.14
1	A	352	LYS	N-CA-C	5.05	117.48	109.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	SER	Peptide
1	A	68	GLU	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	4756	0	4761	133	0
2	A	4	0	0	0	0
3	A	15	0	17	3	0
All	All	4775	0	4778	133	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 14.

All (133) 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:352:LYS:HB3	1:A:370:LYS:HA	1.53	0.90
1:A:584:VAL:O	1:A:587:GLU:N	2.08	0.86
1:A:286:GLY:HA3	1:A:289:GLN:HB2	1.69	0.74
1:A:373:GLN:O	1:A:375:ALA:N	2.26	0.69
1:A:352:LYS:CB	1:A:370:LYS:HA	2.24	0.66
1:A:115:TYR:CE1	3:A:705:DTB:HCR	2.30	0.66
1:A:29:TRP:C	1:A:32:SER:H	2.03	0.66
1:A:282:ILE:HG23	1:A:291:LEU:HD23	1.78	0.66
1:A:535:LEU:HD13	1:A:558:TYR:HE1	1.66	0.61
1:A:351:LEU:O	1:A:351:LEU:HG	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ARG:O	1:A:621:GLU:C	2.42	0.60
1:A:67:PHE:O	1:A:68:GLU:HB2	2.02	0.59
1:A:279:LEU:HG	1:A:279:LEU:O	2.03	0.59
1:A:378:THR:N	1:A:379:PRO:CD	2.66	0.58
1:A:51:LEU:HD12	1:A:51:LEU:O	2.04	0.58
1:A:260:GLN:HA	1:A:263:LYS:HE3	1.84	0.58
1:A:535:LEU:HD11	1:A:543:PRO:HG2	1.86	0.57
1:A:592:TRP:HE3	1:A:593:ARG:N	2.03	0.57
1:A:353:PRO:O	1:A:355:ILE:HG13	2.06	0.56
1:A:438:THR:HA	1:A:441:MET:HB2	1.87	0.56
1:A:480:MET:O	1:A:484:MET:HG3	2.06	0.56
1:A:585:ALA:O	1:A:589:ASP:N	2.37	0.56
1:A:592:TRP:CE3	1:A:593:ARG:HA	2.40	0.56
1:A:354:ARG:NE	1:A:367:LEU:O	2.39	0.55
1:A:578:GLY:HA2	1:A:581:HIS:CD2	2.41	0.55
1:A:377:VAL:C	1:A:379:PRO:HD2	2.30	0.55
1:A:354:ARG:O	1:A:355:ILE:HB	2.07	0.55
1:A:592:TRP:CE3	1:A:593:ARG:N	2.75	0.55
1:A:442:ARG:O	1:A:443:LEU:HB2	2.06	0.55
1:A:372:LEU:HD13	1:A:374:GLU:H	1.72	0.54
1:A:114:LEU:O	1:A:151:VAL:HG22	2.07	0.54
1:A:443:LEU:HD12	1:A:443:LEU:N	2.22	0.54
1:A:115:TYR:CZ	3:A:705:DTB:HCR	2.43	0.54
1:A:72:VAL:HG22	1:A:105:LEU:HD11	1.89	0.54
1:A:190:ARG:NH2	1:A:229:LYS:O	2.41	0.53
1:A:286:GLY:O	1:A:287:ASP:HB3	2.08	0.53
1:A:544:ALA:O	1:A:550:LEU:HD11	2.09	0.52
1:A:550:LEU:HB3	1:A:551:PRO:HD2	1.90	0.52
1:A:243:PHE:HA	1:A:258:LEU:HD13	1.91	0.52
1:A:480:MET:O	1:A:484:MET:CG	2.58	0.52
1:A:350:PRO:HG2	1:A:442:ARG:HH12	1.75	0.51
1:A:592:TRP:CZ2	1:A:596:VAL:HG21	2.46	0.51
1:A:592:TRP:CE3	1:A:592:TRP:C	2.89	0.51
1:A:354:ARG:HH22	1:A:358:ARG:HB3	1.77	0.50
1:A:586:HIS:HA	1:A:589:ASP:HB3	1.93	0.50
1:A:425:HIS:NE2	1:A:602:MET:SD	2.85	0.50
1:A:451:VAL:HG22	1:A:553:MET:HE3	1.94	0.50
1:A:29:TRP:O	1:A:32:SER:HB3	2.12	0.50
1:A:343:THR:HG21	1:A:461:TRP:HE1	1.76	0.50
1:A:373:GLN:O	1:A:373:GLN:HG2	2.10	0.50
1:A:508:TYR:O	1:A:512:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:O	1:A:595:GLN:HG2	2.12	0.49
1:A:304:ARG:O	1:A:307:LEU:HG	2.13	0.49
1:A:418:THR:HG22	1:A:419:ILE:N	2.27	0.49
1:A:585:ALA:O	1:A:589:ASP:HB2	2.12	0.49
1:A:371:LEU:HD11	1:A:445:ASN:HA	1.93	0.49
1:A:471:PHE:HB3	1:A:592:TRP:CZ2	2.48	0.49
1:A:230:SER:HB3	1:A:233:LEU:HD23	1.94	0.49
1:A:592:TRP:CE3	1:A:593:ARG:CA	2.96	0.49
1:A:578:GLY:O	1:A:584:VAL:CG1	2.60	0.49
1:A:442:ARG:HG3	1:A:443:LEU:H	1.77	0.49
1:A:506:ALA:O	1:A:510:ILE:HG12	2.11	0.49
1:A:599:THR:HG23	1:A:602:MET:HE2	1.95	0.49
1:A:591:LEU:O	1:A:595:GLN:N	2.41	0.49
1:A:115:TYR:CE1	1:A:151:VAL:HG21	2.48	0.48
1:A:40:GLN:O	1:A:44:ILE:HG12	2.13	0.48
1:A:286:GLY:O	1:A:287:ASP:CB	2.62	0.48
1:A:343:THR:HG22	1:A:457:LEU:HD22	1.95	0.48
1:A:291:LEU:HD12	1:A:291:LEU:O	2.12	0.48
1:A:621:GLU:HA	1:A:622:TYR:HA	1.63	0.48
1:A:624:LEU:O	1:A:625:GLY:C	2.57	0.48
1:A:259:MET:HE3	1:A:311:PRO:HG3	1.96	0.48
1:A:584:VAL:O	1:A:585:ALA:C	2.55	0.48
1:A:534:GLU:HB3	1:A:540:ILE:HG13	1.95	0.47
1:A:78:MET:HE1	1:A:114:LEU:HD12	1.94	0.47
1:A:437:VAL:O	1:A:441:MET:N	2.43	0.47
1:A:535:LEU:HD13	1:A:558:TYR:CE1	2.48	0.47
1:A:586:HIS:O	1:A:590:GLU:N	2.46	0.47
1:A:542:GLY:O	1:A:544:ALA:N	2.43	0.47
1:A:443:LEU:N	1:A:443:LEU:CD1	2.77	0.46
1:A:519:LEU:HD23	1:A:545:ASN:HB2	1.96	0.46
1:A:420:LEU:HD21	1:A:594:ALA:CB	2.46	0.46
1:A:204:ILE:HG12	1:A:254:MET:HE2	1.98	0.46
1:A:364:ASN:HB3	1:A:549:ASP:HB2	1.97	0.46
1:A:582:TRP:CD1	1:A:583:ARG:H	2.33	0.46
1:A:591:LEU:O	1:A:595:GLN:HG3	2.15	0.46
1:A:420:LEU:HD21	1:A:594:ALA:HB1	1.98	0.46
1:A:337:LEU:HA	1:A:340:ILE:HG22	1.98	0.45
1:A:366:LEU:O	1:A:368:GLN:OE1	2.33	0.45
1:A:619:GLY:CA	1:A:625:GLY:HA2	2.46	0.45
1:A:465:MET:HB2	1:A:495:GLN:HG2	1.97	0.45
1:A:592:TRP:CH2	1:A:596:VAL:HG21	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:CYS:SG	1:A:71:GLU:N	2.90	0.45
1:A:422:GLY:C	1:A:424:PHE:H	2.25	0.44
1:A:236:ASN:OD1	1:A:237:ASN:N	2.50	0.44
1:A:592:TRP:O	1:A:596:VAL:HG23	2.18	0.44
1:A:190:ARG:HD2	1:A:231:LEU:HD13	1.99	0.44
1:A:89:TYR:O	1:A:90:ASP:C	2.61	0.44
1:A:27:GLU:C	1:A:28:SER:O	2.56	0.44
1:A:179:VAL:O	1:A:183:ILE:HG12	2.18	0.43
1:A:352:LYS:HG2	1:A:353:PRO:O	2.17	0.43
1:A:519:LEU:HD22	1:A:519:LEU:HA	1.86	0.43
1:A:592:TRP:C	1:A:592:TRP:CD2	2.96	0.43
1:A:373:GLN:HB2	1:A:445:ASN:OD1	2.18	0.43
1:A:36:GLN:O	1:A:40:GLN:N	2.49	0.43
1:A:90:ASP:O	1:A:91:ASN:OD1	2.36	0.43
1:A:274:SER:OG	1:A:631:ARG:HD3	2.19	0.43
1:A:378:THR:N	1:A:379:PRO:HD2	2.34	0.43
1:A:176:GLU:O	1:A:180:ARG:HG2	2.19	0.42
1:A:328:PHE:CE2	1:A:469:ARG:HB2	2.54	0.42
1:A:356:THR:HG22	1:A:358:ARG:H	1.84	0.42
1:A:427:ILE:HG23	1:A:459:LEU:HG	2.01	0.42
1:A:252:ILE:HD12	1:A:309:GLN:HE21	1.85	0.42
1:A:307:LEU:HD22	1:A:597:VAL:HG11	2.01	0.42
1:A:244:LYS:HE3	1:A:244:LYS:HB2	1.73	0.42
1:A:372:LEU:CD1	1:A:374:GLU:HB2	2.50	0.41
1:A:488:ASP:O	1:A:491:ARG:HB2	2.19	0.41
1:A:584:VAL:HG13	1:A:585:ALA:N	2.34	0.41
1:A:441:MET:HE1	1:A:446:SER:OG	2.20	0.41
1:A:482:GLN:C	1:A:484:MET:N	2.77	0.41
1:A:351:LEU:O	1:A:351:LEU:CG	2.53	0.41
1:A:56:ASN:O	1:A:56:ASN:ND2	2.54	0.41
1:A:88:LEU:HD22	3:A:705:DTB:N1	2.35	0.41
1:A:505:SER:O	1:A:509:ILE:HG12	2.21	0.41
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.85	0.41
1:A:29:TRP:HA	1:A:32:SER:HB2	2.02	0.40
1:A:33:ARG:O	1:A:36:GLN:N	2.54	0.40
1:A:396:VAL:O	1:A:400:LEU:N	2.50	0.40
1:A:42:LYS:O	1:A:46:GLU:HG3	2.21	0.40
1:A:171:ALA:HB1	1:A:203:LEU:HD21	2.04	0.40
1:A:590:GLU:O	1:A:593:ARG:HB3	2.21	0.40
1:A:592:TRP:HE3	1:A:593:ARG:CA	2.35	0.40
1:A:464:VAL:O	1:A:467:PHE:N	2.49	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	590/672 (88%)	536 (91%)	52 (9%)	2 (0%)	36 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	ASP
1	A	378	THR

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	511/584 (88%)	496 (97%)	15 (3%)	37 58

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	MET
1	A	228	LEU
1	A	282	ILE
1	A	368	GLN
1	A	371	LEU
1	A	389	LEU

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Mol	Chain	Res	Type
1	A	441	MET
1	A	514	GLU
1	A	519	LEU
1	A	527	MET
1	A	588	ARG
1	A	592	TRP
1	A	622	TYR
1	A	630	LEU
1	A	631	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	41	GLN
1	A	92	ASN
1	A	128	GLN
1	A	129	ASN
1	A	192	GLN
1	A	206	GLN
1	A	256	GLN
1	A	260	GLN
1	A	309	GLN
1	A	364	ASN
1	A	586	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	DTB	A	705	-	15,15,15	2.51	4 (26%)	16,19,19	2.15	5 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTB	A	705	-	-	5/8/20/20	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	705	DTB	CN-N2	6.54	1.47	1.35
3	A	705	DTB	CN-N1	5.78	1.45	1.35
3	A	705	DTB	CR-N2	-2.54	1.42	1.46
3	A	705	DTB	OI2-C	-2.09	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	705	DTB	CS-CR-N2	4.31	107.67	102.19
3	A	705	DTB	CR-CS-N1	4.17	107.68	102.46
3	A	705	DTB	CS-N1-CN	-3.04	108.33	112.39
3	A	705	DTB	CR-N2-CN	-2.77	108.31	112.38
3	A	705	DTB	CD-CE-CR	-2.21	109.73	113.94

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	705	DTB	CD-CE-CR-N2
3	A	705	DTB	CG-CD-CE-CR
3	A	705	DTB	OI1-C-CA-CB
3	A	705	DTB	CE-CD-CG-CB
3	A	705	DTB	OI2-C-CA-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	DTB	3	0

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	596/672 (88%)	0.91	89 (14%) 5 9	99, 139, 204, 240	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	608	PRO	10.9
1	A	610	CYS	7.2
1	A	156	PRO	7.2
1	A	607	LEU	6.5
1	A	611	LEU	6.4
1	A	556	ILE	6.4
1	A	559	ALA	6.3
1	A	353	PRO	5.8
1	A	564	ILE	5.7
1	A	68	GLU	5.7
1	A	562	ALA	5.6
1	A	560	ALA	5.5
1	A	157	HIS	5.4
1	A	609	ARG	5.3
1	A	563	ILE	5.2
1	A	604	GLU	5.0
1	A	159	LEU	4.9
1	A	141	ALA	4.8
1	A	568	LEU	4.8
1	A	606	LYS	4.8
1	A	292	LEU	4.7
1	A	603	LEU	4.6
1	A	143	VAL	4.6
1	A	566	THR	4.5
1	A	612	TRP	4.4
1	A	570	LEU	4.3
1	A	480	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	155	ARG	4.1
1	A	283	ASP	4.0
1	A	105	LEU	4.0
1	A	374	GLU	4.0
1	A	615	SER	3.8
1	A	136	LEU	3.8
1	A	605	ARG	3.7
1	A	377	VAL	3.7
1	A	284	SER	3.7
1	A	569	MET	3.7
1	A	282	ILE	3.6
1	A	544	ALA	3.6
1	A	635	ARG	3.4
1	A	247	GLY	3.3
1	A	540	ILE	3.3
1	A	614	ARG	3.3
1	A	314	GLU	3.2
1	A	194	SER	3.2
1	A	279	LEU	3.2
1	A	572	LEU	3.1
1	A	481	ILE	3.0
1	A	483	LYS	2.9
1	A	378	THR	2.8
1	A	106	VAL	2.8
1	A	482	GLN	2.8
1	A	538	THR	2.8
1	A	291	LEU	2.7
1	A	567	LEU	2.7
1	A	552	PHE	2.7
1	A	166	PRO	2.7
1	A	243	PHE	2.6
1	A	138	ALA	2.6
1	A	351	LEU	2.6
1	A	613	PRO	2.6
1	A	542	GLY	2.6
1	A	137	LEU	2.5
1	A	306	ILE	2.5
1	A	139	ARG	2.5
1	A	154	TYR	2.5
1	A	561	PHE	2.5
1	A	493	CYS	2.4
1	A	539	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLU	2.4
1	A	361	PRO	2.3
1	A	34	ASP	2.3
1	A	491	ARG	2.3
1	A	285	SER	2.2
1	A	72	VAL	2.2
1	A	321	LYS	2.2
1	A	100	GLU	2.2
1	A	555	SER	2.1
1	A	280	THR	2.1
1	A	468	ALA	2.1
1	A	497	ALA	2.1
1	A	573	LEU	2.1
1	A	471	PHE	2.1
1	A	98	LEU	2.1
1	A	101	ALA	2.1
1	A	315	LEU	2.1
1	A	421	GLY	2.0
1	A	99	MET	2.0
1	A	327	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(Å ²)	Q<0.9
2	BA	A	702	1/1	-0.18	0.26	154,154,154,154	1
2	BA	A	704	1/1	0.78	0.07	110,110,110,110	1
2	BA	A	701	1/1	0.82	0.19	154,154,154,154	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BA	A	703	1/1	0.84	0.26	154,154,154,154	1
3	DTB	A	705	15/15	0.84	0.15	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.