



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:56 PM UTC

PDB ID : 5IWK / pdb_00005iwk
Title : Structure of Transient Receptor Potential (TRP) channel TRPV6
Authors : Saotome, K.; Singh, A.K.; Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on : 2016-03-22
Resolution : 3.25 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

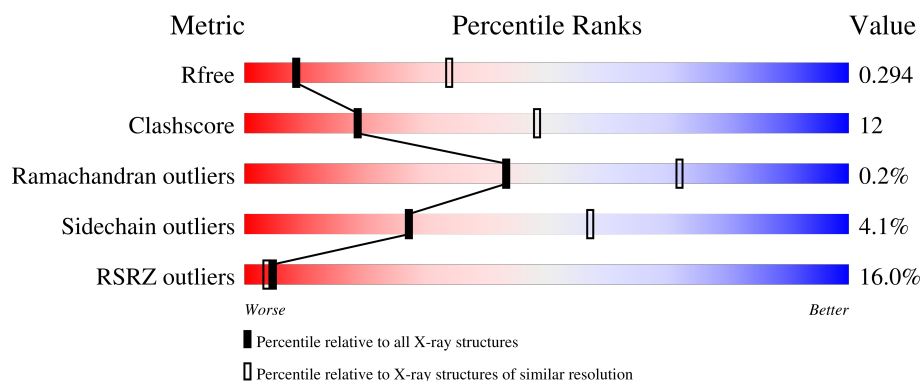
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	14% 64% 21% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4743 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	594	Total	C	N	O	S	0	0	0
			4727	3054	793	848	32			

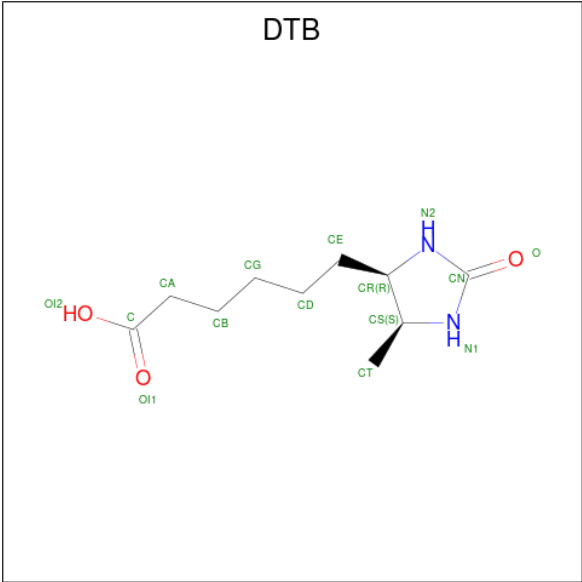
There are 7 discrepancies between the modelled and reference sequences:

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 CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

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

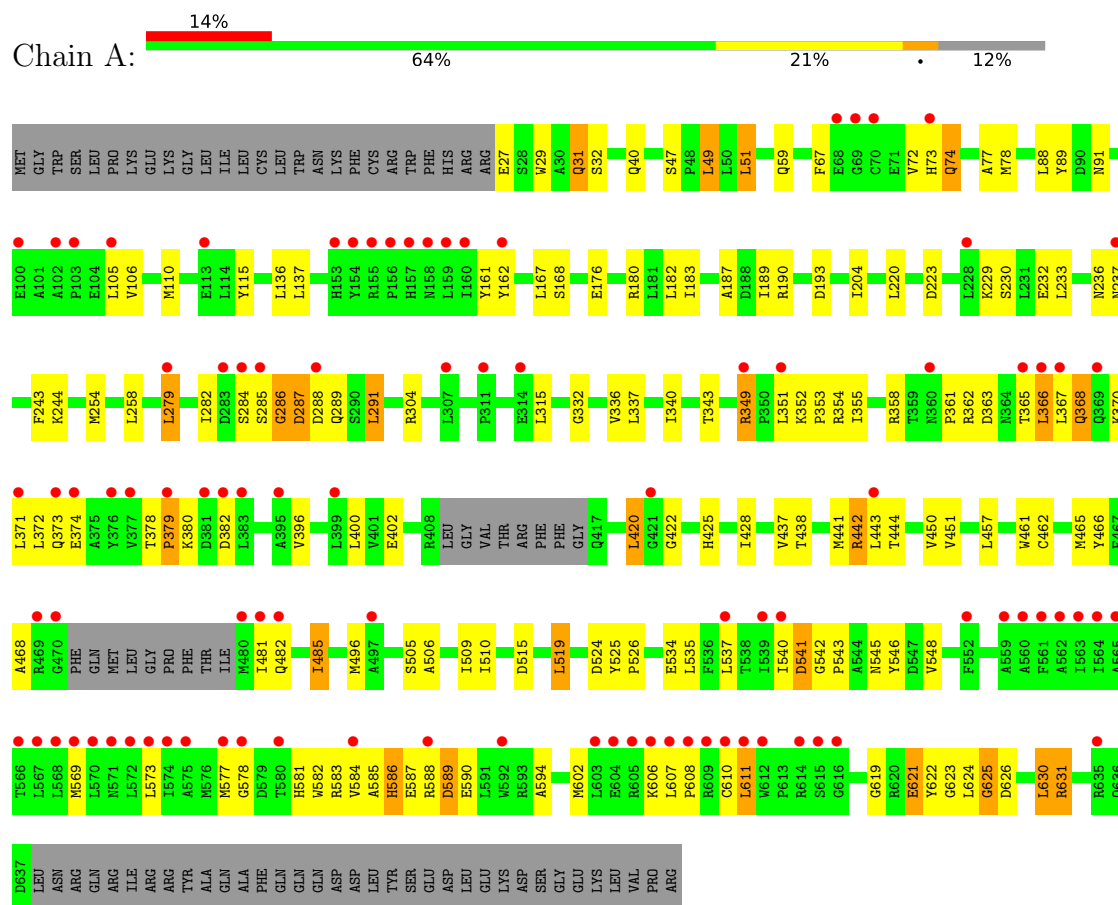


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	10	2	3	0	0

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	143.82Å 143.82Å 113.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 3.25 49.46 – 3.25	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.46-3.25) 96.0 (49.46-3.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.261 , 0.288 (Not available) , 0.294	Depositor DCC
R_{free} test set	928 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	130.7	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.4	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	0.88	EDS
Total number of atoms	4743	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: CA, 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	0.66	3/4834 (0.1%)	0.91	24/6568 (0.4%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	625	GLY	N-CA	-28.77	1.03	1.45
1	A	353	PRO	N-CD	-7.40	1.37	1.47
1	A	372	LEU	CA-C	-5.50	1.45	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	GLY	N-CA-C	26.77	176.63	113.18
1	A	589	ASP	N-CA-C	13.03	125.50	111.03
1	A	286	GLY	N-CA-C	-11.98	96.29	112.82
1	A	422	GLY	N-CA-C	-9.62	92.72	112.34
1	A	541	ASP	N-CA-C	-9.48	95.84	109.96
1	A	622	TYR	N-CA-C	8.28	134.18	111.00
1	A	380	LYS	N-CA-C	-8.18	101.78	112.41
1	A	373	GLN	N-CA-C	-8.11	100.70	110.44
1	A	481	ILE	N-CA-C	7.42	118.16	110.36
1	A	289	GLN	N-CA-C	7.26	121.74	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	LEU	N-CA-C	-6.88	96.15	110.80
1	A	287	ASP	N-CA-C	-6.87	103.79	111.28
1	A	379	PRO	CB-CA-C	-6.63	100.61	111.56
1	A	374	GLU	N-CA-C	-6.42	104.70	113.30
1	A	31	GLN	N-CA-C	-6.37	104.34	111.28
1	A	291	LEU	N-CA-C	-6.18	104.62	111.36
1	A	622	TYR	CB-CA-C	-5.95	98.80	110.10
1	A	588	ARG	N-CA-C	-5.76	105.00	111.28
1	A	372	LEU	CB-CA-C	-5.75	98.28	109.68
1	A	626	ASP	N-CA-C	-5.48	106.45	114.39
1	A	353	PRO	N-CA-C	5.44	119.24	111.13
1	A	288	ASP	N-CA-C	-5.36	104.66	113.50
1	A	451	VAL	CB-CA-C	-5.16	108.89	114.35
1	A	379	PRO	N-CA-C	5.05	122.88	112.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	621	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	4727	0	4726	112	1
2	A	1	0	0	0	0
3	A	15	0	17	2	0
All	All	4743	0	4743	113	1

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 12.

All (113) 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:284:SER:O	1:A:285:SER:OG	1.67	1.11
1:A:582:TRP:CD1	1:A:584:VAL:HG23	1.85	1.10
1:A:582:TRP:HD1	1:A:584:VAL:HG23	1.05	1.10
1:A:578:GLY:HA2	1:A:581:HIS:CD2	1.92	1.05
1:A:284:SER:C	1:A:285:SER:HG	1.86	0.81
1:A:352:LYS:H	1:A:370:LYS:CB	2.01	0.73
1:A:582:TRP:HD1	1:A:584:VAL:CG2	1.95	0.73
1:A:578:GLY:CA	1:A:581:HIS:CD2	2.74	0.67
1:A:586:HIS:CD2	1:A:586:HIS:C	2.72	0.67
1:A:537:LEU:HD23	1:A:569:MET:HE1	1.76	0.66
1:A:110:MET:HB2	1:A:115:TYR:O	1.98	0.63
1:A:88:LEU:HD23	1:A:89:TYR:CE1	2.33	0.62
1:A:425:HIS:NE2	1:A:602:MET:SD	2.71	0.61
1:A:284:SER:O	1:A:285:SER:CB	2.45	0.60
1:A:78:MET:SD	1:A:115:TYR:HE2	2.23	0.60
1:A:437:VAL:O	1:A:441:MET:N	2.32	0.60
1:A:115:TYR:CE1	3:A:702:DTB:HCR	2.37	0.60
1:A:590:GLU:O	1:A:594:ALA:N	2.28	0.58
1:A:438:THR:HA	1:A:441:MET:HB2	1.86	0.58
1:A:585:ALA:O	1:A:589:ASP:N	2.37	0.57
1:A:535:LEU:CD2	1:A:542:GLY:HA2	2.35	0.57
1:A:525:TYR:N	1:A:526:PRO:CD	2.68	0.56
1:A:623:GLY:O	1:A:624:LEU:HD22	2.05	0.56
1:A:358:ARG:HA	1:A:361:PRO:HD2	1.87	0.56
1:A:370:LYS:O	1:A:371:LEU:HD22	2.07	0.54
1:A:505:SER:HA	1:A:525:TYR:HE1	1.72	0.54
1:A:190:ARG:NH2	1:A:229:LYS:O	2.36	0.54
1:A:442:ARG:C	1:A:444:THR:H	2.16	0.53
1:A:351:LEU:HA	1:A:370:LYS:CB	2.39	0.53
1:A:535:LEU:HD22	1:A:542:GLY:HA2	1.90	0.53
1:A:578:GLY:O	1:A:581:HIS:HD2	1.92	0.53
1:A:105:LEU:O	1:A:106:VAL:C	2.52	0.52
1:A:47:SER:OG	1:A:74:GLN:NE2	2.42	0.52
1:A:519:LEU:HD11	1:A:543:PRO:HB3	1.93	0.51
1:A:204:ILE:HG12	1:A:254:MET:HE2	1.92	0.51
1:A:378:THR:OG1	1:A:382:ASP:N	2.44	0.51
1:A:578:GLY:C	1:A:581:HIS:HD2	2.18	0.51
1:A:89:TYR:CD1	1:A:89:TYR:N	2.79	0.51
1:A:450:VAL:HG23	1:A:509:ILE:HG22	1.93	0.51
1:A:363:ASP:OD2	1:A:363:ASP:N	2.41	0.50
1:A:167:LEU:HA	1:A:182:LEU:HD13	1.94	0.49
1:A:545:ASN:CG	1:A:548:VAL:HG22	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:MET:SD	1:A:115:TYR:CE2	3.05	0.49
1:A:623:GLY:C	1:A:624:LEU:HD22	2.38	0.49
1:A:27:GLU:O	1:A:27:GLU:HG3	2.13	0.48
1:A:534:GLU:HB3	1:A:540:ILE:HG12	1.95	0.48
1:A:586:HIS:CD2	1:A:587:GLU:N	2.82	0.48
1:A:362:ARG:CB	1:A:365:THR:HG23	2.44	0.48
1:A:230:SER:HB3	1:A:233:LEU:HD23	1.96	0.48
1:A:582:TRP:CG	1:A:583:ARG:N	2.82	0.47
1:A:337:LEU:HA	1:A:340:ILE:HG22	1.96	0.47
1:A:402:GLU:OE2	1:A:425:HIS:ND1	2.47	0.47
1:A:72:VAL:C	1:A:74:GLN:H	2.22	0.47
1:A:506:ALA:O	1:A:510:ILE:HG12	2.14	0.47
1:A:606:LYS:O	1:A:607:LEU:C	2.57	0.47
1:A:582:TRP:CD1	1:A:584:VAL:H	2.33	0.47
1:A:236:ASN:OD1	1:A:237:ASN:N	2.48	0.46
1:A:40:GLN:HA	1:A:77:ALA:HB3	1.97	0.46
1:A:72:VAL:HG13	1:A:73:HIS:N	2.31	0.46
1:A:367:LEU:HD12	1:A:367:LEU:N	2.31	0.46
1:A:189:ILE:HD11	1:A:223:ASP:HA	1.98	0.46
1:A:482:GLN:O	1:A:485:ILE:N	2.48	0.46
1:A:443:LEU:HD12	1:A:443:LEU:N	2.31	0.46
1:A:279:LEU:HD21	1:A:315:LEU:HD13	1.98	0.45
1:A:183:ILE:HD13	1:A:187:ALA:HB3	1.98	0.45
1:A:49:LEU:HD12	1:A:49:LEU:O	2.16	0.45
1:A:466:TYR:C	1:A:468:ALA:H	2.24	0.45
1:A:161:TYR:OH	1:A:193:ASP:OD2	2.32	0.45
1:A:354:ARG:O	1:A:355:ILE:C	2.60	0.45
1:A:29:TRP:O	1:A:32:SER:HB3	2.16	0.45
1:A:619:GLY:C	1:A:625:GLY:HA3	2.41	0.44
1:A:540:ILE:HG22	1:A:541:ASP:O	2.17	0.44
1:A:220:LEU:HD21	1:A:232:GLU:HG3	1.99	0.44
1:A:462:CYS:O	1:A:465:MET:HG2	2.17	0.44
1:A:578:GLY:O	1:A:581:HIS:CD2	2.70	0.44
1:A:343:THR:HG22	1:A:457:LEU:HD22	1.99	0.43
1:A:349:ARG:HH11	1:A:349:ARG:HG2	1.83	0.43
1:A:366:LEU:CD2	1:A:515:ASP:HB3	2.48	0.43
1:A:358:ARG:CA	1:A:361:PRO:HD2	2.49	0.43
1:A:352:LYS:N	1:A:370:LYS:CB	2.77	0.43
1:A:243:PHE:HA	1:A:258:LEU:HD13	2.00	0.42
1:A:162:TYR:O	1:A:168:SER:OG	2.30	0.42
1:A:582:TRP:CD1	1:A:584:VAL:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:PRO:HG2	1:A:611:LEU:HD23	2.01	0.42
1:A:51:LEU:HD12	1:A:51:LEU:O	2.20	0.42
1:A:286:GLY:O	1:A:287:ASP:C	2.61	0.42
1:A:535:LEU:HD23	1:A:540:ILE:HB	2.00	0.42
1:A:89:TYR:O	1:A:91:ASN:N	2.52	0.42
1:A:525:TYR:HB3	1:A:526:PRO:HD3	2.02	0.42
1:A:106:VAL:HG13	1:A:136:LEU:HD22	2.01	0.42
1:A:244:LYS:HB2	1:A:244:LYS:HE3	1.91	0.42
1:A:578:GLY:C	1:A:581:HIS:CD2	2.96	0.42
1:A:40:GLN:HB2	1:A:78:MET:HE2	2.01	0.41
1:A:610:CYS:SG	1:A:611:LEU:HD22	2.60	0.41
1:A:621:GLU:H	1:A:623:GLY:H	1.68	0.41
1:A:540:ILE:O	1:A:541:ASP:C	2.61	0.41
1:A:466:TYR:C	1:A:468:ALA:N	2.78	0.41
1:A:343:THR:HG21	1:A:461:TRP:HE1	1.85	0.41
1:A:358:ARG:C	1:A:361:PRO:HD2	2.45	0.41
1:A:396:VAL:O	1:A:400:LEU:N	2.51	0.41
1:A:354:ARG:HB2	1:A:368:GLN:HA	2.02	0.41
1:A:428:ILE:HD12	1:A:428:ILE:HA	1.94	0.41
1:A:573:LEU:HB3	1:A:577:MET:HE3	2.02	0.41
1:A:630:LEU:HD12	1:A:631:ARG:N	2.36	0.41
1:A:291:LEU:HA	1:A:291:LEU:HD12	1.78	0.41
1:A:176:GLU:O	1:A:180:ARG:HG2	2.22	0.40
1:A:279:LEU:CD2	1:A:630:LEU:HB2	2.52	0.40
3:A:702:DTB:HCE2	3:A:702:DTB:HCT3	1.94	0.40
1:A:608:PRO:HG2	1:A:611:LEU:CD2	2.52	0.40
1:A:367:LEU:N	1:A:367:LEU:CD1	2.84	0.40
1:A:545:ASN:O	1:A:546:TYR:CD1	2.75	0.40
1:A:332:GLY:O	1:A:336:VAL:HG23	2.22	0.40
1:A:621:GLU:N	1:A:623:GLY:H	2.18	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:OE1	1:A:67:PHE:CE1[8_556]	1.91	0.29

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	571/672 (85%)	534 (94%)	36 (6%)	1 (0%)	43 72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	PRO

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	507/584 (87%)	486 (96%)	21 (4%)	27 57

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	49	LEU
1	A	51	LEU
1	A	74	GLN
1	A	137	LEU
1	A	279	LEU
1	A	282	ILE
1	A	304	ARG
1	A	349	ARG
1	A	366	LEU

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Mol	Chain	Res	Type
1	A	368	GLN
1	A	420	LEU
1	A	442	ARG
1	A	485	ILE
1	A	496	MET
1	A	519	LEU
1	A	524	ASP
1	A	586	HIS
1	A	611	LEU
1	A	630	LEU
1	A	631	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	41	GLN
1	A	74	GLN
1	A	92	ASN
1	A	129	ASN
1	A	192	GLN
1	A	264	HIS
1	A	581	HIS
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 2 ligands modelled in this entry, 1 is 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	702	-	15,15,15	0.65	0	16,19,19	1.18	1 (6%)

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	702	-	-	5/8/20/20	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	DTB	OI2-C-CA	2.29	121.24	114.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	DTB	CE-CD-CG-CB
3	A	702	DTB	CD-CE-CR-N2
3	A	702	DTB	OI2-C-CA-CB
3	A	702	DTB	OI1-C-CA-CB
3	A	702	DTB	CG-CD-CE-CR

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	DTB	2	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	594/672 (88%)	0.87	95 (15%) 5 3	84, 113, 170, 214	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	566	THR	9.1
1	A	156	PRO	8.4
1	A	609	ARG	7.4
1	A	610	CYS	7.0
1	A	608	PRO	6.8
1	A	570	LEU	6.7
1	A	154	TYR	6.3
1	A	113	GLU	5.7
1	A	567	LEU	5.5
1	A	374	GLU	5.4
1	A	562	ALA	5.4
1	A	560	ALA	5.2
1	A	367	LEU	5.2
1	A	607	LEU	5.1
1	A	480	MET	5.0
1	A	563	ILE	4.8
1	A	155	ARG	4.7
1	A	382	ASP	4.7
1	A	70	CYS	4.6
1	A	569	MET	4.6
1	A	564	ILE	4.6
1	A	349	ARG	4.5
1	A	573	LEU	4.4
1	A	158	ASN	4.3
1	A	159	LEU	4.3
1	A	559	ALA	4.2
1	A	605	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	611	LEU	4.1
1	A	470	GLY	4.1
1	A	565	ALA	4.1
1	A	157	HIS	4.0
1	A	606	LYS	4.0
1	A	604	GLU	4.0
1	A	379	PRO	4.0
1	A	366	LEU	3.9
1	A	540	ILE	3.7
1	A	614	ARG	3.6
1	A	279	LEU	3.4
1	A	481	ILE	3.4
1	A	100	GLU	3.3
1	A	383	LEU	3.3
1	A	237	ASN	3.3
1	A	160	ILE	3.2
1	A	365	THR	3.1
1	A	102	ALA	3.1
1	A	285	SER	3.0
1	A	351	LEU	2.9
1	A	568	LEU	2.9
1	A	283	ASP	2.9
1	A	577	MET	2.9
1	A	578	GLY	2.8
1	A	73	HIS	2.8
1	A	584	VAL	2.8
1	A	572	LEU	2.7
1	A	284	SER	2.6
1	A	635	ARG	2.6
1	A	575	ALA	2.5
1	A	561	PHE	2.5
1	A	314	GLU	2.4
1	A	360	ASN	2.4
1	A	162	TYR	2.4
1	A	371	LEU	2.4
1	A	482	GLN	2.4
1	A	153	HIS	2.4
1	A	311	PRO	2.3
1	A	539	ILE	2.3
1	A	592	TRP	2.3
1	A	571	ASN	2.3
1	A	68	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	552	PHE	2.3
1	A	369	GLN	2.3
1	A	373	GLN	2.3
1	A	69	GLY	2.2
1	A	616	GLY	2.2
1	A	399	LEU	2.2
1	A	497	ALA	2.2
1	A	615	SER	2.2
1	A	612	TRP	2.2
1	A	228	LEU	2.2
1	A	288	ASP	2.2
1	A	574	ILE	2.1
1	A	103	PRO	2.1
1	A	469	ARG	2.1
1	A	307	LEU	2.1
1	A	588	ARG	2.1
1	A	537	LEU	2.1
1	A	381	ASP	2.1
1	A	421	GLY	2.1
1	A	376	TYR	2.0
1	A	377	VAL	2.0
1	A	105	LEU	2.0
1	A	443	LEU	2.0
1	A	395	ALA	2.0
1	A	580	THR	2.0
1	A	603	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	DTB	A	702	15/15	0.92	0.17	92,103,113,122	0
2	CA	A	701	1/1	0.98	0.13	94,94,94,94	1

6.5 Other polymers [i](#)

There are no such residues in this entry.