



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:39 PM UTC

PDB ID : 5IWP / pdb_00005iwp
Title : Structure of Transient Receptor Potential (TRP) channel TRPV6 in the presence of calcium
Authors : Saotome, K.; Singh, A.K.; Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on : 2016-03-22
Resolution : 3.65 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

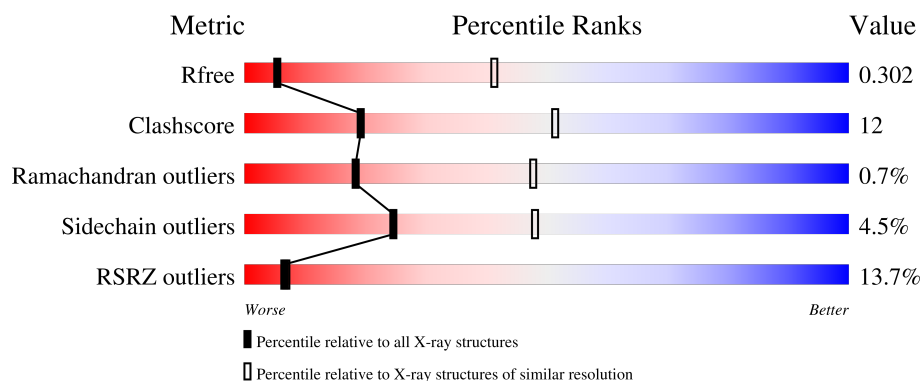
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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	12% 64% 19% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4735 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	591	Total	C	N	O	S	0	0	0
			4717	3049	792	844	32			

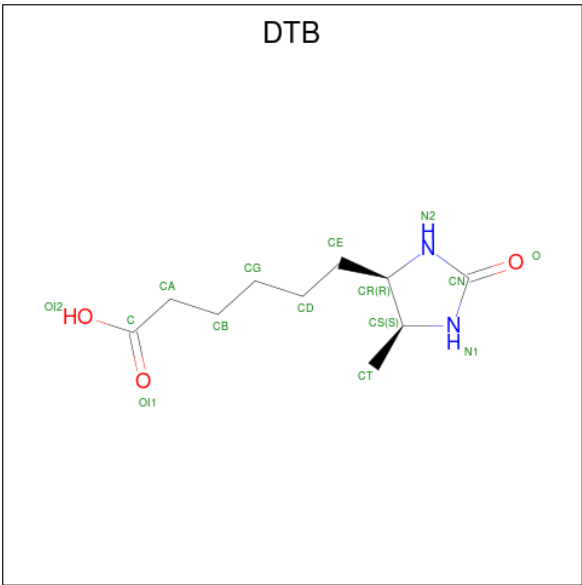
There are 7 discrepancies between the modelled and reference sequences:

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	3	Total	Ca	0	0
			3	3		

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

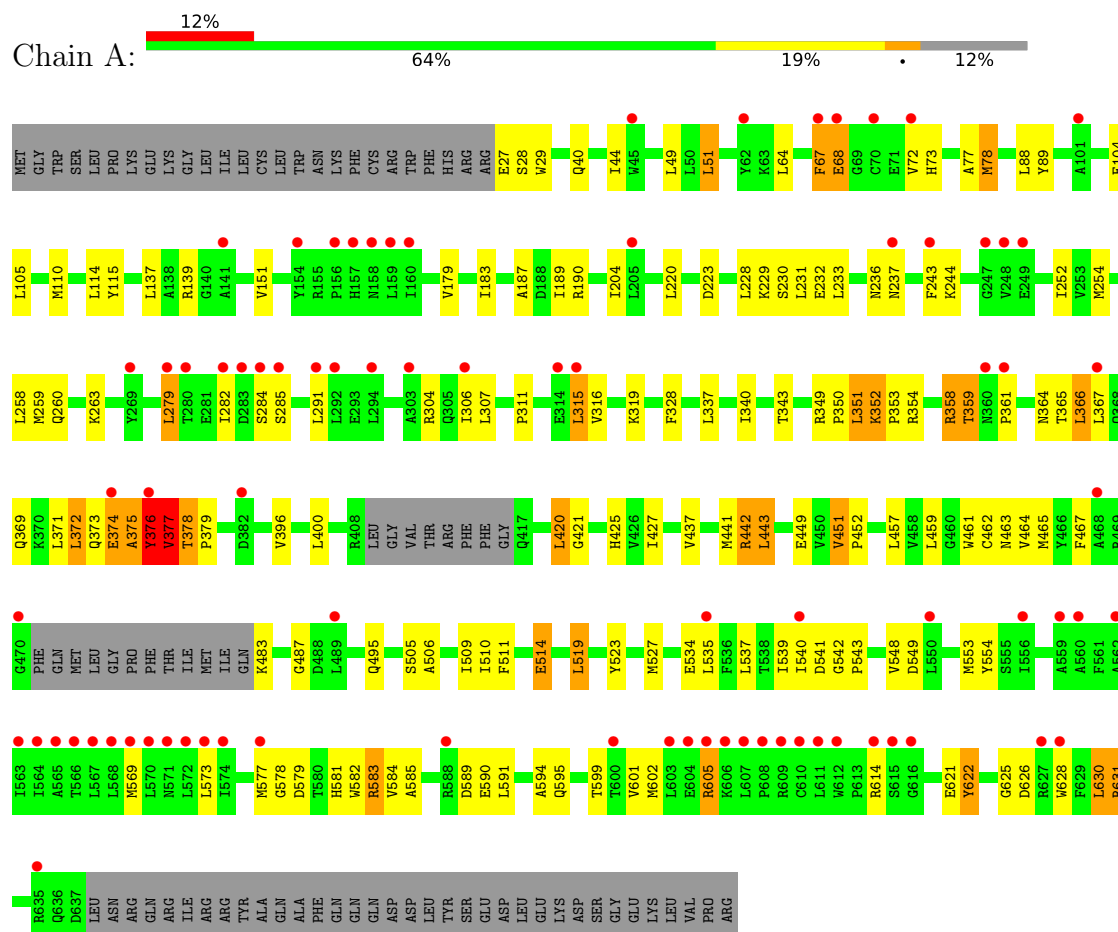


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	10	2	3	0	0

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 – 3.65 49.56 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.56-3.65) 99.8 (49.56-3.65)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.273 , 0.283 0.302 , 0.302	Depositor DCC
R_{free} test set	692 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	142.3	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.0	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	0.83	EDS
Total number of atoms	4735	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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	0.29	3/4824 (0.1%)	0.70	19/6553 (0.3%)

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	372	LEU	CA-C	-10.61	1.39	1.52
1	A	372	LEU	C-O	-7.71	1.14	1.23
1	A	67	PHE	CA-C	5.32	1.58	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	THR	N-CA-C	-17.45	92.12	113.41
1	A	378	THR	N-CA-C	13.34	128.66	109.71
1	A	359	THR	N-CA-CB	10.81	126.26	110.47
1	A	67	PHE	N-CA-C	-10.54	90.01	108.13
1	A	67	PHE	CB-CA-C	9.50	124.11	110.24
1	A	68	GLU	N-CA-C	-8.54	87.09	111.00
1	A	375	ALA	N-CA-C	-8.52	92.65	110.80
1	A	372	LEU	CA-C-O	-8.49	111.50	121.44
1	A	589	ASP	N-CA-C	8.10	123.71	112.04
1	A	315	LEU	N-CA-C	7.17	119.17	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	ARG	N-CA-C	7.13	119.13	111.36
1	A	68	GLU	N-CA-CB	7.10	122.57	110.50
1	A	579	ASP	N-CA-C	-6.89	105.15	113.97
1	A	372	LEU	N-CA-C	5.96	118.75	109.52
1	A	378	THR	N-CA-CB	-5.68	97.70	109.28
1	A	451	VAL	CB-CA-C	-5.59	108.42	114.35
1	A	358	ARG	CB-CA-C	-5.50	99.96	110.57
1	A	585	ALA	N-CA-C	-5.39	105.57	111.82
1	A	377	VAL	N-CA-C	5.30	120.37	109.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	LEU	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	4717	0	4734	110	0
2	A	3	0	0	0	0
3	A	15	0	17	3	0
All	All	4735	0	4751	111	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 12.

All (111) 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:376:TYR:O	1:A:377:VAL:HG22	1.41	1.19
1:A:375:ALA:HA	1:A:376:TYR:O	1.68	0.92
1:A:376:TYR:O	1:A:377:VAL:CG2	2.25	0.81
1:A:315:LEU:O	1:A:315:LEU:HD12	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:GLY:HA2	1:A:581:HIS:HD2	1.49	0.78
1:A:375:ALA:HA	1:A:376:TYR:C	2.18	0.69
1:A:114:LEU:O	1:A:151:VAL:HG22	1.93	0.68
1:A:351:LEU:HB3	1:A:352:LYS:HA	1.75	0.67
1:A:578:GLY:HA2	1:A:581:HIS:CD2	2.30	0.65
1:A:115:TYR:CE1	3:A:704:DTB:HCR	2.32	0.65
1:A:420:LEU:H	1:A:421:GLY:HA3	1.60	0.64
1:A:366:LEU:HD12	1:A:366:LEU:H	1.63	0.63
1:A:183:ILE:HD13	1:A:187:ALA:HB3	1.81	0.63
1:A:519:LEU:HD11	1:A:543:PRO:HB3	1.83	0.61
1:A:354:ARG:NE	1:A:367:LEU:O	2.34	0.60
1:A:373:GLN:HB2	1:A:375:ALA:HB3	1.83	0.60
1:A:365:THR:HG22	1:A:367:LEU:H	1.67	0.59
1:A:537:LEU:HD13	1:A:569:MET:HE1	1.82	0.59
1:A:543:PRO:O	1:A:554:TYR:OH	2.15	0.57
1:A:378:THR:HG23	1:A:378:THR:O	2.04	0.57
1:A:540:ILE:HG22	1:A:542:GLY:H	1.71	0.56
1:A:190:ARG:NH2	1:A:229:LYS:O	2.41	0.54
1:A:315:LEU:HD12	1:A:315:LEU:C	2.32	0.53
1:A:441:MET:HE3	1:A:452:PRO:HG3	1.90	0.53
1:A:243:PHE:HA	1:A:258:LEU:HD13	1.90	0.52
1:A:367:LEU:HB3	1:A:369:GLN:HG3	1.91	0.52
1:A:115:TYR:CZ	3:A:704:DTB:HCR	2.45	0.52
1:A:343:THR:HG21	1:A:461:TRP:HE1	1.74	0.52
1:A:590:GLU:O	1:A:594:ALA:N	2.32	0.51
1:A:364:ASN:ND2	1:A:549:ASP:OD1	2.37	0.51
1:A:437:VAL:O	1:A:441:MET:N	2.39	0.51
1:A:282:ILE:HG23	1:A:291:LEU:HD23	1.93	0.51
1:A:506:ALA:O	1:A:510:ILE:HG12	2.10	0.50
1:A:584:VAL:HG22	1:A:584:VAL:O	2.10	0.50
1:A:284:SER:HB2	1:A:285:SER:HB2	1.94	0.50
1:A:72:VAL:HG22	1:A:105:LEU:HD11	1.94	0.49
1:A:351:LEU:CB	1:A:352:LYS:HA	2.40	0.49
1:A:591:LEU:O	1:A:595:GLN:HG3	2.12	0.49
1:A:190:ARG:HD2	1:A:231:LEU:HD13	1.93	0.49
1:A:443:LEU:HD12	1:A:443:LEU:O	2.12	0.49
1:A:230:SER:HB3	1:A:233:LEU:HD23	1.94	0.49
1:A:582:TRP:CD1	1:A:583:ARG:H	2.30	0.49
1:A:630:LEU:HD12	1:A:631:ARG:N	2.28	0.49
1:A:304:ARG:O	1:A:307:LEU:HG	2.13	0.49
1:A:425:HIS:NE2	1:A:602:MET:SD	2.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:O	1:A:443:LEU:HB3	2.13	0.48
1:A:40:GLN:O	1:A:44:ILE:HG12	2.14	0.48
1:A:316:VAL:HA	1:A:319:LYS:HD3	1.96	0.47
1:A:337:LEU:HA	1:A:340:ILE:HG22	1.97	0.47
1:A:451:VAL:HG13	1:A:553:MET:SD	2.54	0.47
1:A:28:SER:OG	1:A:29:TRP:N	2.48	0.46
1:A:78:MET:HE1	1:A:114:LEU:HD12	1.97	0.46
1:A:599:THR:HG23	1:A:602:MET:HE2	1.95	0.46
1:A:441:MET:CE	1:A:452:PRO:HG3	2.45	0.46
1:A:461:TRP:O	1:A:464:VAL:HB	2.15	0.46
1:A:343:THR:HG22	1:A:457:LEU:HD22	1.98	0.46
1:A:372:LEU:HB2	1:A:373:GLN:HA	1.97	0.46
1:A:115:TYR:CE1	1:A:151:VAL:HG21	2.51	0.46
1:A:236:ASN:OD1	1:A:237:ASN:N	2.47	0.46
1:A:67:PHE:HA	1:A:68:GLU:HA	1.77	0.46
1:A:88:LEU:HD23	1:A:89:TYR:CE1	2.51	0.46
1:A:505:SER:O	1:A:509:ILE:HG12	2.16	0.46
1:A:315:LEU:CD1	1:A:319:LYS:HD2	2.47	0.45
1:A:51:LEU:HD12	1:A:51:LEU:O	2.17	0.45
1:A:73:HIS:NE2	1:A:104:GLU:HG3	2.32	0.44
1:A:220:LEU:HD21	1:A:232:GLU:HG3	2.00	0.44
1:A:352:LYS:HB2	1:A:353:PRO:HD2	1.98	0.44
1:A:373:GLN:HB2	1:A:375:ALA:N	2.33	0.44
1:A:625:GLY:HA2	1:A:626:ASP:HA	1.63	0.44
1:A:291:LEU:HD12	1:A:291:LEU:O	2.17	0.43
1:A:315:LEU:HD11	1:A:319:LYS:HD2	2.00	0.43
1:A:582:TRP:C	1:A:584:VAL:H	2.26	0.43
1:A:350:PRO:HG2	1:A:442:ARG:HH12	1.82	0.43
1:A:483:LYS:O	1:A:487:GLY:N	2.50	0.43
1:A:523:TYR:CE1	1:A:527:MET:HG2	2.54	0.43
1:A:27:GLU:HA	1:A:28:SER:HA	1.73	0.43
1:A:204:ILE:HG12	1:A:254:MET:HE2	2.00	0.43
1:A:358:ARG:C	1:A:361:PRO:HD2	2.44	0.43
1:A:534:GLU:HB3	1:A:539:ILE:CG2	2.49	0.43
1:A:614:ARG:HD3	1:A:628:TRP:CE2	2.54	0.43
1:A:64:LEU:O	1:A:68:GLU:O	2.36	0.42
1:A:427:ILE:HG23	1:A:459:LEU:HG	2.00	0.42
1:A:621:GLU:N	1:A:622:TYR:O	2.52	0.42
1:A:252:ILE:HD13	1:A:306:ILE:HD13	2.01	0.42
1:A:244:LYS:HE3	1:A:244:LYS:HB2	1.74	0.42
1:A:459:LEU:O	1:A:463:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:VAL:O	1:A:605:ARG:HG3	2.19	0.42
1:A:279:LEU:HD12	1:A:279:LEU:C	2.45	0.42
1:A:49:LEU:HD12	1:A:49:LEU:O	2.20	0.42
1:A:539:ILE:HG23	1:A:540:ILE:N	2.33	0.42
1:A:465:MET:SD	1:A:495:GLN:HG2	2.59	0.42
1:A:40:GLN:HA	1:A:77:ALA:HB3	2.01	0.42
1:A:315:LEU:O	1:A:319:LYS:HG3	2.19	0.42
1:A:462:CYS:O	1:A:465:MET:HG2	2.20	0.41
1:A:573:LEU:HB3	1:A:577:MET:HE3	2.02	0.41
1:A:179:VAL:O	1:A:183:ILE:HG12	2.20	0.41
1:A:328:PHE:CZ	1:A:467:PHE:HA	2.55	0.41
1:A:366:LEU:HD12	1:A:366:LEU:N	2.31	0.41
1:A:396:VAL:O	1:A:400:LEU:N	2.51	0.41
1:A:543:PRO:HB2	1:A:554:TYR:CZ	2.55	0.41
1:A:189:ILE:HD11	1:A:223:ASP:HA	2.02	0.41
1:A:260:GLN:HA	1:A:263:LYS:HE3	2.03	0.41
1:A:366:LEU:HD13	1:A:514:GLU:HB3	2.03	0.41
1:A:511:PHE:HA	1:A:514:GLU:HG2	2.02	0.41
1:A:110:MET:HB2	1:A:115:TYR:O	2.21	0.40
1:A:373:GLN:HA	1:A:374:GLU:HB2	2.03	0.40
1:A:259:MET:HE3	1:A:311:PRO:HG3	2.04	0.40
1:A:535:LEU:CD2	1:A:542:GLY:HA2	2.51	0.40
3:A:704:DTB:HCE2	3:A:704:DTB:HCT3	1.90	0.40
1:A:375:ALA:CA	1:A:376:TYR:C	2.90	0.40
1:A:441:MET:HG2	1:A:449:GLU:HA	2.03	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	585/672 (87%)	537 (92%)	44 (8%)	4 (1%)	18	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	TYR
1	A	377	VAL
1	A	379	PRO
1	A	583	ARG

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	508/584 (87%)	485 (96%)	23 (4%)	24	48

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	78	MET
1	A	137	LEU
1	A	139	ARG
1	A	228	LEU
1	A	279	LEU
1	A	349	ARG
1	A	352	LYS
1	A	359	THR
1	A	366	LEU
1	A	371	LEU
1	A	374	GLU
1	A	376	TYR
1	A	420	LEU
1	A	442	ARG
1	A	443	LEU
1	A	514	GLU
1	A	519	LEU
1	A	541	ASP
1	A	548	VAL
1	A	622	TYR

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Mol	Chain	Res	Type
1	A	630	LEU
1	A	631	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	192	GLN
1	A	227	HIS
1	A	256	GLN
1	A	289	GLN
1	A	309	GLN
1	A	373	GLN

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, 3 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	704	-	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	704	-	-	4/8/20/20	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	DTB	CN-N2	6.54	1.47	1.35
3	A	704	DTB	CN-N1	5.77	1.45	1.35
3	A	704	DTB	CR-N2	-2.47	1.42	1.46
3	A	704	DTB	OI2-C	-2.11	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	DTB	CS-CR-N2	4.30	107.66	102.19
3	A	704	DTB	CR-CS-N1	4.18	107.69	102.46
3	A	704	DTB	CS-N1-CN	-3.04	108.33	112.39
3	A	704	DTB	CR-N2-CN	-2.81	108.25	112.38
3	A	704	DTB	CD-CE-CR	-2.24	109.68	113.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	DTB	CD-CE-CR-N2
3	A	704	DTB	OI2-C-CA-CB
3	A	704	DTB	OI1-C-CA-CB
3	A	704	DTB	CG-CD-CE-CR

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	704	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	591/672 (87%)	0.85	81 (13%) 6 7	80, 131, 187, 213	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	566	THR	9.0
1	A	608	PRO	8.5
1	A	570	LEU	8.3
1	A	569	MET	8.3
1	A	283	ASP	8.2
1	A	607	LEU	7.2
1	A	615	SER	6.8
1	A	614	ARG	6.8
1	A	567	LEU	6.7
1	A	604	GLU	6.7
1	A	284	SER	6.7
1	A	562	ALA	6.6
1	A	156	PRO	6.6
1	A	563	ILE	6.3
1	A	154	TYR	6.2
1	A	609	ARG	5.6
1	A	159	LEU	5.5
1	A	573	LEU	5.4
1	A	282	ILE	5.3
1	A	560	ALA	5.2
1	A	568	LEU	5.1
1	A	577	MET	5.0
1	A	610	CYS	4.9
1	A	279	LEU	4.9
1	A	564	ILE	4.7
1	A	556	ILE	4.7
1	A	247	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	612	TRP	4.3
1	A	249	GLU	4.2
1	A	627	ARG	4.2
1	A	540	ILE	4.0
1	A	248	VAL	4.0
1	A	565	ALA	4.0
1	A	606	LYS	3.9
1	A	68	GLU	3.8
1	A	572	LEU	3.8
1	A	603	LEU	3.8
1	A	571	ASN	3.8
1	A	294	LEU	3.7
1	A	314	GLU	3.7
1	A	376	TYR	3.7
1	A	62	TYR	3.6
1	A	635	ARG	3.6
1	A	280	THR	3.6
1	A	616	GLY	3.5
1	A	292	LEU	3.5
1	A	559	ALA	3.5
1	A	374	GLU	3.5
1	A	470	GLY	3.3
1	A	574	ILE	3.3
1	A	611	LEU	3.2
1	A	628	TRP	3.2
1	A	315	LEU	3.0
1	A	605	ARG	3.0
1	A	285	SER	2.8
1	A	291	LEU	2.8
1	A	367	LEU	2.8
1	A	243	PHE	2.8
1	A	160	ILE	2.7
1	A	101	ALA	2.7
1	A	72	VAL	2.6
1	A	303	ALA	2.6
1	A	237	ASN	2.5
1	A	157	HIS	2.5
1	A	361	PRO	2.5
1	A	67	PHE	2.5
1	A	141	ALA	2.5
1	A	382	ASP	2.5
1	A	360	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	269	TYR	2.4
1	A	306	ILE	2.3
1	A	158	ASN	2.2
1	A	588	ARG	2.2
1	A	45	TRP	2.2
1	A	600	THR	2.2
1	A	535	LEU	2.2
1	A	70	CYS	2.1
1	A	489	LEU	2.1
1	A	205	LEU	2.0
1	A	550	LEU	2.0
1	A	468	ALA	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	CA	A	702	1/1	0.20	0.19	25,25,25,25	1
3	DTB	A	704	15/15	0.81	0.18	77,77,77,77	0
2	CA	A	703	1/1	0.94	0.44	25,25,25,25	1
2	CA	A	701	1/1	0.94	0.07	25,25,25,25	1

6.5 Other polymers [i](#)

There are no such residues in this entry.