



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:43 PM EDT

PDB ID : 6D7P / pdb_00006d7p
Title : Crystal Structure of Rat TRPV6*-Y466A
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Deposited on : 2018-04-25
Resolution : 3.37 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

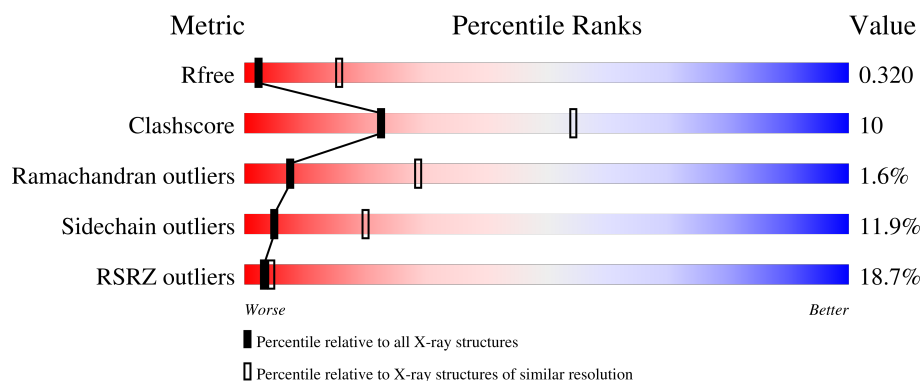
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	17% 63% 24% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4862 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	610	Total	C	N	O	S	0	0	0
			4845	3137	811	863	34			

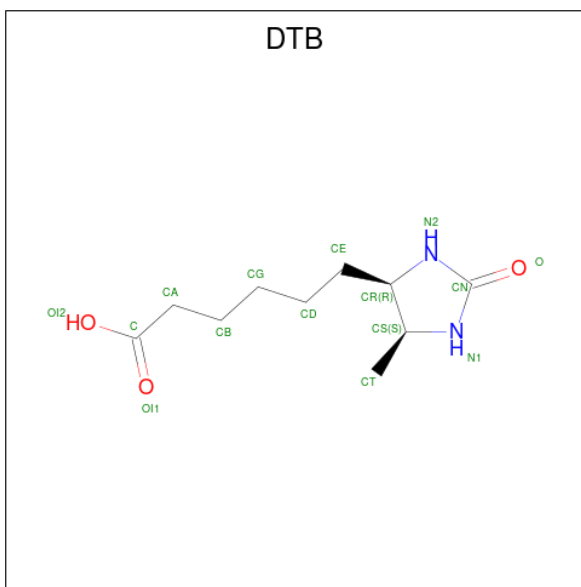
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	TYR	ILE	conflict	UNP Q9R186
A	92	ASN	LEU	conflict	UNP Q9R186
A	96	GLN	MET	conflict	UNP Q9R186
A	466	ALA	TYR	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	2	Total	Ca	0	0
			2	2		

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

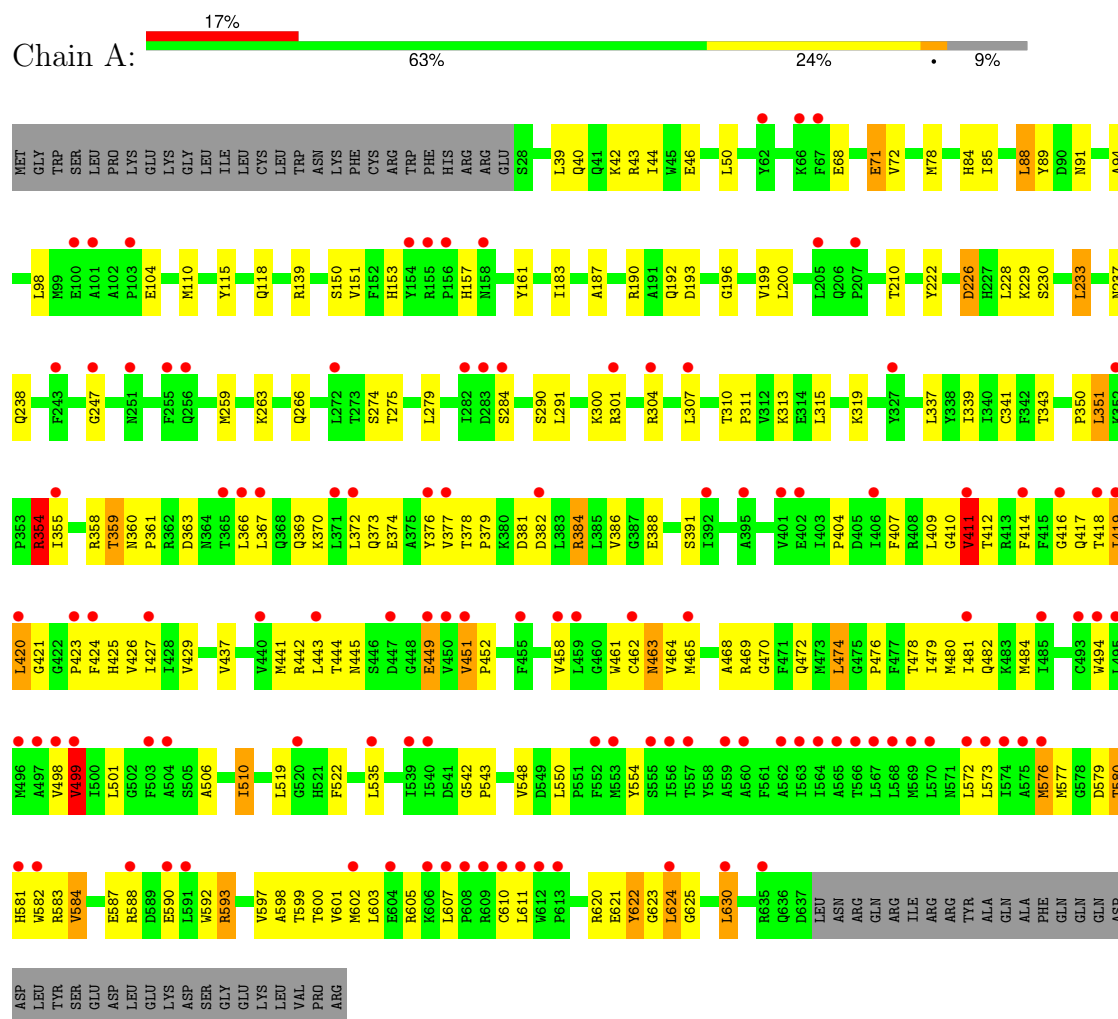


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	10	2	3	0	0

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	146.05Å 146.05Å 116.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	116.49 – 3.37 116.49 – 3.37	Depositor EDS
% Data completeness (in resolution range)	94.2 (116.49-3.37) 94.4 (116.49-3.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.295 , 0.310 0.312 , 0.320	Depositor DCC
R_{free} test set	831 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	141.5	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4862	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	0.15	0/4957	0.39	0/6738

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4845	0	4866	101	0
2	A	2	0	0	0	0
3	A	15	0	17	2	0
All	All	4862	0	4883	102	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 10.

All (102) 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:584:VAL:HA	1:A:587:GLU:HB2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASP:OD1	1:A:226:ASP:N	2.22	0.73
1:A:469:ARG:NH1	1:A:599:THR:OG1	2.23	0.71
1:A:535:LEU:HD11	1:A:542:GLY:HA2	1.75	0.69
1:A:543:PRO:O	1:A:554:TYR:OH	2.06	0.69
1:A:441:MET:HE3	1:A:452:PRO:HG2	1.75	0.69
1:A:43:ARG:NH1	1:A:46:GLU:OE1	2.28	0.66
1:A:358:ARG:O	1:A:360:ASN:N	2.27	0.66
1:A:343:THR:HG21	1:A:461:TRP:HE1	1.60	0.66
1:A:451:VAL:HG13	1:A:452:PRO:HD3	1.79	0.65
1:A:411:VAL:HG13	1:A:412:THR:H	1.60	0.65
1:A:427:ILE:HD11	1:A:463:ASN:HB2	1.79	0.65
1:A:376:TYR:CG	1:A:377:VAL:N	2.66	0.64
1:A:484:MET:SD	1:A:576:MET:HE1	2.38	0.63
1:A:284:SER:HA	1:A:290:SER:HB2	1.80	0.63
1:A:425:HIS:CD2	1:A:463:ASN:HD21	2.16	0.63
1:A:279:LEU:HD11	1:A:315:LEU:HD22	1.82	0.61
1:A:42:LYS:NZ	1:A:46:GLU:OE2	2.27	0.61
1:A:484:MET:SD	1:A:576:MET:CE	2.89	0.61
1:A:259:MET:HE3	1:A:311:PRO:HG3	1.83	0.60
1:A:421:GLY:HA3	1:A:425:HIS:CG	2.38	0.59
1:A:247:GLY:HA3	1:A:291:LEU:HD21	1.84	0.59
1:A:463:ASN:O	1:A:463:ASN:ND2	2.35	0.58
1:A:602:MET:HA	1:A:605:ARG:HB2	1.85	0.58
1:A:480:MET:HG2	1:A:588:ARG:NH1	2.19	0.57
1:A:378:THR:HA	1:A:381:ASP:HB3	1.87	0.56
1:A:590:GLU:HA	1:A:593:ARG:HD2	1.88	0.55
1:A:161:TYR:OH	1:A:193:ASP:OD2	2.24	0.54
1:A:412:THR:O	1:A:416:GLY:N	2.33	0.54
1:A:374:GLU:OE2	1:A:445:ASN:ND2	2.41	0.54
1:A:414:PHE:O	1:A:418:THR:N	2.38	0.54
1:A:419:ILE:HB	1:A:602:MET:HB3	1.90	0.53
1:A:419:ILE:O	1:A:421:GLY:N	2.42	0.53
1:A:506:ALA:O	1:A:510:ILE:HG12	2.10	0.52
1:A:230:SER:HB3	1:A:233:LEU:HD23	1.92	0.52
1:A:301:ARG:NH2	1:A:587:GLU:OE1	2.43	0.52
1:A:376:TYR:CD2	1:A:377:VAL:N	2.77	0.52
1:A:622:TYR:O	1:A:624:LEU:N	2.35	0.51
1:A:442:ARG:HG3	1:A:443:LEU:H	1.76	0.51
1:A:421:GLY:HA3	1:A:425:HIS:CD2	2.45	0.51
1:A:419:ILE:HG23	1:A:599:THR:HA	1.92	0.51
1:A:183:ILE:HA	1:A:187:ALA:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:SER:HA	1:A:153:HIS:CE1	2.47	0.49
1:A:404:PRO:HA	1:A:407:PHE:HB3	1.95	0.49
1:A:192:GLN:NE2	1:A:196:GLY:O	2.41	0.48
1:A:468:ALA:HB1	1:A:474:LEU:HD13	1.95	0.48
1:A:378:THR:HB	1:A:382:ASP:HB2	1.94	0.48
1:A:40:GLN:O	1:A:44:ILE:HG12	2.14	0.47
1:A:307:LEU:HD13	1:A:597:VAL:HG21	1.95	0.47
1:A:266:GLN:OE1	1:A:274:SER:OG	2.29	0.47
1:A:354:ARG:HA	1:A:369:GLN:OE1	2.14	0.47
1:A:470:GLY:H	1:A:592:TRP:HE1	1.63	0.46
1:A:339:ILE:O	1:A:343:THR:HG23	2.15	0.46
3:A:703:DTB:HCT1	3:A:703:DTB:HCE2	1.55	0.46
1:A:84:HIS:CE1	1:A:110:MET:HG2	2.50	0.46
1:A:494:TRP:O	1:A:498:VAL:HG23	2.16	0.46
1:A:310:THR:HA	1:A:313:LYS:HG2	1.97	0.45
1:A:620:ARG:O	1:A:621:GLU:HB3	2.15	0.45
1:A:43:ARG:HD3	1:A:43:ARG:HA	1.78	0.45
1:A:442:ARG:C	1:A:444:THR:H	2.23	0.45
1:A:359:THR:O	1:A:363:ASP:HA	2.17	0.45
1:A:190:ARG:NH2	1:A:229:LYS:O	2.34	0.44
1:A:279:LEU:HD22	1:A:630:LEU:HB2	1.99	0.44
1:A:463:ASN:HD22	1:A:463:ASN:C	2.25	0.44
1:A:423:PRO:HB3	1:A:482:GLN:NE2	2.32	0.44
1:A:474:LEU:O	1:A:478:THR:HG23	2.17	0.44
1:A:157:HIS:H	1:A:157:HIS:CD2	2.34	0.44
1:A:300:LYS:HD3	1:A:300:LYS:HA	1.82	0.44
1:A:469:ARG:HH11	1:A:599:THR:HG1	1.60	0.44
1:A:89:TYR:C	1:A:91:ASN:HD22	2.26	0.44
1:A:351:LEU:O	1:A:370:LYS:HA	2.17	0.44
1:A:110:MET:HE2	1:A:118:GLN:OE1	2.18	0.43
1:A:110:MET:HE3	1:A:115:TYR:HB3	2.01	0.43
1:A:50:LEU:HD12	1:A:85:ILE:HG13	2.00	0.43
1:A:310:THR:HG23	1:A:311:PRO:HD3	2.00	0.43
1:A:498:VAL:HG12	1:A:499:VAL:H	1.83	0.43
1:A:476:PRO:HD3	1:A:592:TRP:CD2	2.54	0.43
1:A:88:LEU:HG	3:A:703:DTB:HN2	1.82	0.43
1:A:190:ARG:H	1:A:190:ARG:HG2	1.52	0.43
1:A:350:PRO:HG3	1:A:384:ARG:HH12	1.84	0.42
1:A:437:VAL:O	1:A:441:MET:N	2.50	0.42
1:A:104:GLU:OE1	1:A:104:GLU:N	2.41	0.42
1:A:498:VAL:O	1:A:499:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:SER:HA	1:A:290:SER:CB	2.49	0.42
1:A:304:ARG:HD2	1:A:590:GLU:HB3	2.02	0.42
1:A:597:VAL:O	1:A:601:VAL:HG23	2.20	0.42
1:A:237:ASN:OD1	1:A:238:GLN:N	2.53	0.41
1:A:183:ILE:HG21	1:A:222:TYR:CD1	2.55	0.41
1:A:319:LYS:HB3	1:A:600:THR:HG21	2.02	0.41
1:A:115:TYR:CE1	1:A:151:VAL:HG11	2.55	0.41
1:A:461:TRP:HA	1:A:464:VAL:HG23	2.03	0.41
1:A:462:CYS:O	1:A:465:MET:HG2	2.20	0.41
1:A:584:VAL:O	1:A:588:ARG:HG2	2.21	0.41
1:A:71:GLU:CD	1:A:71:GLU:H	2.26	0.41
1:A:424:PHE:C	1:A:426:VAL:H	2.28	0.41
1:A:442:ARG:NH1	1:A:449:GLU:OE2	2.54	0.41
1:A:580:THR:H	1:A:584:VAL:HG21	1.86	0.41
1:A:419:ILE:HG12	1:A:598:ALA:O	2.21	0.40
1:A:581:HIS:CD2	1:A:583:ARG:HG2	2.56	0.40
1:A:388:GLU:O	1:A:391:SER:OG	2.33	0.40
1:A:94:ALA:O	1:A:98:LEU:HG	2.21	0.40
1:A:358:ARG:O	1:A:361:PRO:HD2	2.21	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	608/672 (90%)	550 (90%)	48 (8%)	10 (2%)	7 29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	PRO
1	A	411	VAL

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Mol	Chain	Res	Type
1	A	420	LEU
1	A	359	THR
1	A	577	MET
1	A	354	ARG
1	A	410	GLY
1	A	623	GLY
1	A	499	VAL
1	A	625	GLY

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	520/583 (89%)	458 (88%)	62 (12%)	5 20

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	68	GLU
1	A	71	GLU
1	A	72	VAL
1	A	78	MET
1	A	88	LEU
1	A	139	ARG
1	A	199	VAL
1	A	200	LEU
1	A	210	THR
1	A	226	ASP
1	A	228	LEU
1	A	233	LEU
1	A	263	LYS
1	A	275	THR
1	A	337	LEU
1	A	341	CYS
1	A	351	LEU

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Mol	Chain	Res	Type
1	A	354	ARG
1	A	355	ILE
1	A	366	LEU
1	A	367	LEU
1	A	372	LEU
1	A	373	GLN
1	A	384	ARG
1	A	386	VAL
1	A	409	LEU
1	A	411	VAL
1	A	417	GLN
1	A	419	ILE
1	A	420	LEU
1	A	429	VAL
1	A	449	GLU
1	A	451	VAL
1	A	458	VAL
1	A	463	ASN
1	A	472	GLN
1	A	474	LEU
1	A	479	ILE
1	A	481	ILE
1	A	499	VAL
1	A	501	LEU
1	A	510	ILE
1	A	519	LEU
1	A	522	PHE
1	A	548	VAL
1	A	550	LEU
1	A	572	LEU
1	A	573	LEU
1	A	576	MET
1	A	579	ASP
1	A	580	THR
1	A	582	TRP
1	A	584	VAL
1	A	593	ARG
1	A	603	LEU
1	A	607	LEU
1	A	610	CYS
1	A	611	LEU
1	A	622	TYR

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Mol	Chain	Res	Type
1	A	624	LEU
1	A	630	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	206	GLN
1	A	260	GLN
1	A	425	HIS
1	A	445	ASN
1	A	463	ASN
1	A	482	GLN
1	A	581	HIS

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 3 ligands modelled in this entry, 2 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	703	-	15,15,15	2.83	3 (20%)	16,19,19	2.33	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	703	-	-	5/8/20/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	DTB	CN-N2	7.42	1.48	1.35
3	A	703	DTB	CN-N1	7.21	1.48	1.35
3	A	703	DTB	O-CN	-2.11	1.18	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	DTB	CR-CS-N1	4.59	108.21	102.46
3	A	703	DTB	CS-CR-N2	4.33	107.70	102.19
3	A	703	DTB	CT-CS-N1	-3.89	103.63	111.86
3	A	703	DTB	CS-N1-CN	-3.07	108.29	112.39
3	A	703	DTB	CR-N2-CN	-3.07	107.88	112.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	DTB	CD-CE-CR-N2
3	A	703	DTB	CD-CE-CR-CS
3	A	703	DTB	OI2-C-CA-CB
3	A	703	DTB	OI1-C-CA-CB
3	A	703	DTB	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	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	610/672 (90%)	1.10	114 (18%) 3 4	81, 123, 169, 188	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	CYS	8.0
1	A	462	CYS	7.8
1	A	569	MET	7.4
1	A	570	LEU	7.2
1	A	573	LEU	7.2
1	A	485	ILE	6.8
1	A	493	CYS	6.8
1	A	376	TYR	6.8
1	A	499	VAL	6.7
1	A	556	ILE	6.7
1	A	497	ALA	6.1
1	A	100	GLU	5.3
1	A	563	ILE	5.1
1	A	455	PHE	5.1
1	A	459	LEU	5.1
1	A	367	LEU	5.0
1	A	553	MET	4.9
1	A	608	PRO	4.8
1	A	576	MET	4.7
1	A	372	LEU	4.7
1	A	371	LEU	4.6
1	A	567	LEU	4.3
1	A	496	MET	4.3
1	A	566	THR	4.3
1	A	635	ARG	4.3
1	A	575	ALA	4.2
1	A	572	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	564	ILE	4.2
1	A	559	ALA	3.9
1	A	420	LEU	3.9
1	A	609	ARG	3.8
1	A	355	ILE	3.7
1	A	560	ALA	3.6
1	A	154	TYR	3.6
1	A	443	LEU	3.6
1	A	557	THR	3.5
1	A	607	LEU	3.5
1	A	67	PHE	3.5
1	A	451	VAL	3.4
1	A	591	LEU	3.4
1	A	604	GLU	3.4
1	A	568	LEU	3.3
1	A	243	PHE	3.2
1	A	602	MET	3.2
1	A	402	GLU	3.2
1	A	458	VAL	3.2
1	A	103	PRO	3.1
1	A	540	ILE	3.1
1	A	365	THR	3.1
1	A	424	PHE	3.1
1	A	582	TRP	3.1
1	A	256	GLN	3.0
1	A	419	ILE	3.0
1	A	498	VAL	2.9
1	A	552	PHE	2.8
1	A	465	MET	2.8
1	A	156	PRO	2.8
1	A	307	LEU	2.8
1	A	401	VAL	2.8
1	A	247	GLY	2.8
1	A	588	ARG	2.8
1	A	503	PHE	2.7
1	A	158	ASN	2.7
1	A	352	LYS	2.7
1	A	447	ASP	2.7
1	A	205	LEU	2.7
1	A	423	PRO	2.6
1	A	450	VAL	2.6
1	A	327	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	427	ILE	2.6
1	A	255	PHE	2.6
1	A	624	LEU	2.6
1	A	440	VAL	2.6
1	A	494	TRP	2.5
1	A	62	TYR	2.5
1	A	611	LEU	2.5
1	A	504	ALA	2.5
1	A	207	PRO	2.5
1	A	284	SER	2.5
1	A	66	LYS	2.5
1	A	481	ILE	2.5
1	A	282	ILE	2.4
1	A	495	LEU	2.4
1	A	539	ILE	2.4
1	A	565	ALA	2.4
1	A	101	ALA	2.3
1	A	283	ASP	2.3
1	A	366	LEU	2.3
1	A	630	LEU	2.3
1	A	581	HIS	2.3
1	A	449	GLU	2.3
1	A	574	ILE	2.3
1	A	406	ILE	2.2
1	A	272	LEU	2.2
1	A	395	ALA	2.2
1	A	612	TRP	2.2
1	A	555	SER	2.2
1	A	304	ARG	2.2
1	A	382	ASP	2.2
1	A	411	VAL	2.1
1	A	392	ILE	2.1
1	A	301	ARG	2.1
1	A	520	GLY	2.1
1	A	155	ARG	2.1
1	A	377	VAL	2.1
1	A	416	GLY	2.1
1	A	251	ASN	2.1
1	A	414	PHE	2.1
1	A	418	THR	2.0
1	A	606	LYS	2.0
1	A	562	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	613	PRO	2.0
1	A	590	GLU	2.0
1	A	535	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(Å ²)	Q<0.9
2	CA	A	702	1/1	0.79	0.08	132,132,132,132	1
3	DTB	A	703	15/15	0.93	0.15	118,118,118,118	0
2	CA	A	701	1/1	0.98	0.12	129,129,129,129	1

6.5 Other polymers [i](#)

There are no such residues in this entry.