



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2017 – 05:35 AM EDT

PDB ID : 5WO6
Title : Crystal Structure of Transient Receptor Potential (TRP) channel TRPV6cryst
Authors : Singh, A.K.; Saotome, K.; Sobolevsky, A.I.
Deposited on : unknown
Resolution : 3.31 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

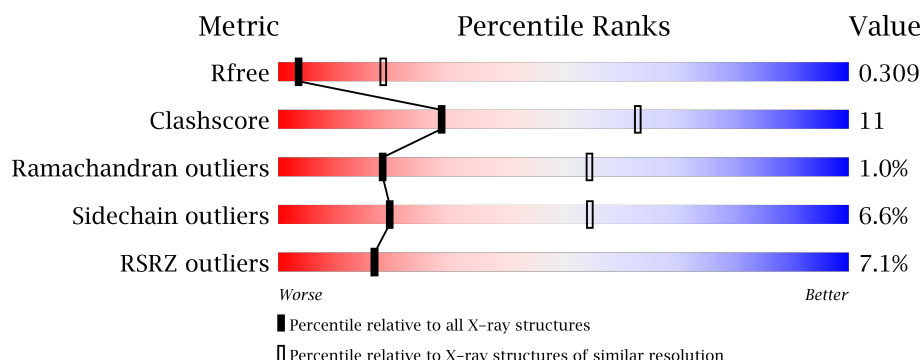
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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}	100719	1002 (3.38-3.26)
Clashscore	112137	1066 (3.38-3.26)
Ramachandran outliers	110173	1048 (3.38-3.26)
Sidechain outliers	110143	1047 (3.38-3.26)
RSRZ outliers	101464	1007 (3.38-3.26)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	668	<div> <div>6%</div> <div>66%</div> <div>22%</div> <div>• 10%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4822 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	602	Total	C	N	O	S	0	0	0
			4806	3111	805	856	34			

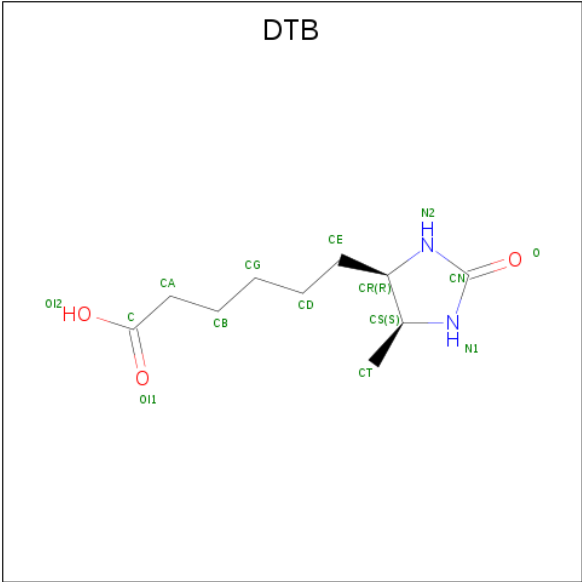
There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CALCIUM ION (three-letter code: 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 (three-letter code: DTB) (formula: C₁₀H₁₈N₂O₃).

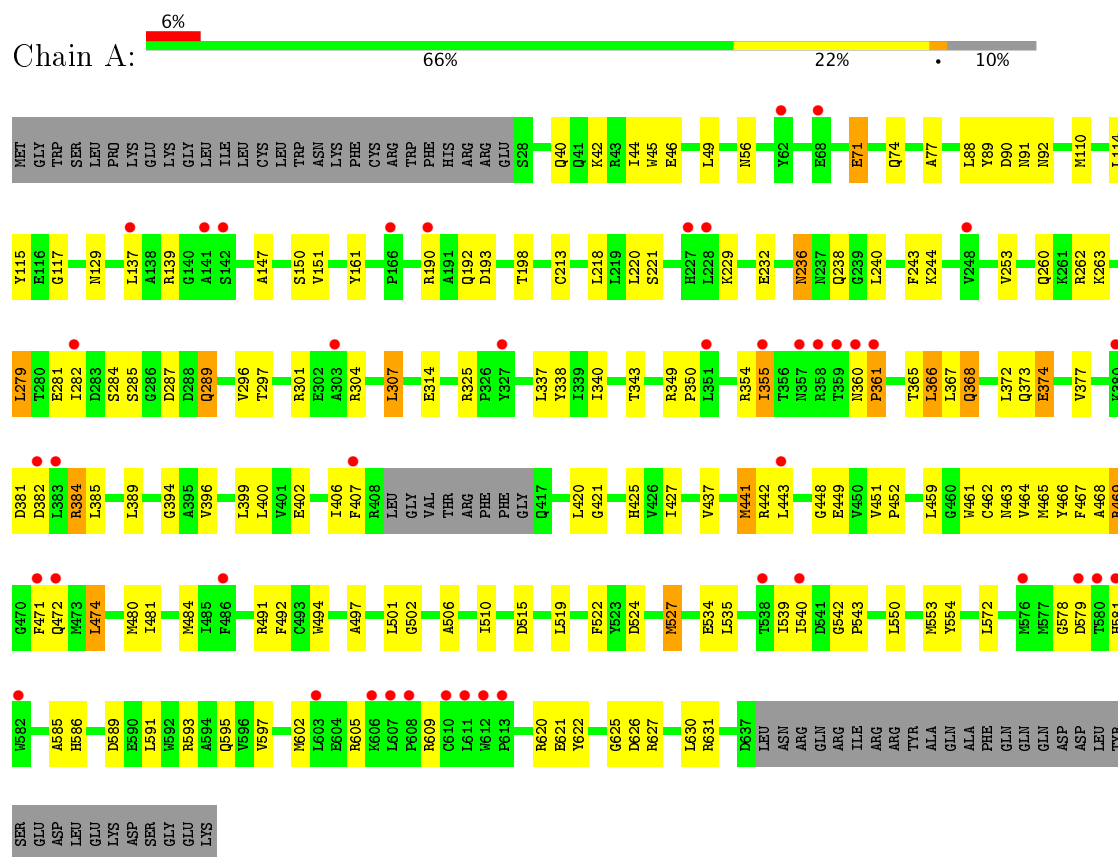


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	10	2	3		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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	145.62Å 145.62Å 114.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.91 – 3.31 49.91 – 3.31	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.91-3.31) 85.9 (49.91-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.287 , 0.314 0.280 , 0.309	Depositor DCC
R_{free} test set	815 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	122.9	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 93.9	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	0.88	EDS
Total number of atoms	4822	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: DTB, 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	0.35	1/4917 (0.0%)	0.48	4/6680 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	PRO	N-CD	16.89	1.71	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	PRO	CA-N-CD	-8.86	99.10	111.50
1	A	361	PRO	N-CA-CB	8.30	113.26	103.30
1	A	360	ASN	C-N-CD	5.90	140.80	128.40
1	A	307	LEU	CA-CB-CG	5.68	128.37	115.30

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	4806	0	4831	104	0
2	A	1	0	0	0	0
3	A	15	0	17	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4822	0	4848	106	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 11.

All (106) 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:361:PRO:N	1:A:361:PRO:CD	1.71	1.35
1:A:451:VAL:HG13	1:A:452:PRO:HD3	1.40	1.00
1:A:451:VAL:CG1	1:A:452:PRO:HD3	1.97	0.94
1:A:461:TRP:O	1:A:464:VAL:HG12	1.72	0.90
1:A:540:ILE:HG22	1:A:542:GLY:H	1.44	0.81
1:A:115:TYR:CE1	3:A:702:DTB:HCR	2.21	0.75
1:A:451:VAL:HG13	1:A:452:PRO:CD	2.16	0.72
1:A:365:THR:HG23	1:A:367:LEU:HD12	1.71	0.71
1:A:451:VAL:CG1	1:A:452:PRO:CD	2.71	0.69
1:A:365:THR:HG23	1:A:367:LEU:CD1	2.24	0.68
1:A:464:VAL:HA	1:A:467:PHE:HD1	1.59	0.68
1:A:425:HIS:NE2	1:A:602:MET:SD	2.62	0.67
1:A:451:VAL:HG23	1:A:553:MET:CE	2.24	0.66
1:A:114:LEU:O	1:A:151:VAL:HG22	1.94	0.66
1:A:366:LEU:HD22	1:A:515:ASP:H	1.60	0.64
1:A:420:LEU:H	1:A:421:GLY:HA3	1.63	0.64
1:A:406:ILE:HD11	1:A:407:PHE:CE2	2.33	0.64
1:A:402:GLU:OE2	1:A:425:HIS:ND1	2.34	0.61
1:A:110:MET:HE3	1:A:115:TYR:HB3	1.83	0.61
1:A:190:ARG:NH2	1:A:229:LYS:O	2.33	0.61
1:A:464:VAL:HA	1:A:467:PHE:CD1	2.36	0.60
1:A:343:THR:HG21	1:A:461:TRP:HE1	1.67	0.60
1:A:385:LEU:O	1:A:389:LEU:HD13	2.03	0.59
1:A:301:ARG:O	1:A:304:ARG:NH1	2.37	0.58
1:A:543:PRO:O	1:A:554:TYR:OH	2.16	0.57
1:A:117:GLY:HA3	1:A:147:ALA:HA	1.87	0.57
1:A:325:ARG:HH21	1:A:471:PHE:HA	1.69	0.56
1:A:519:LEU:HD22	1:A:550:LEU:HD21	1.89	0.54
3:A:702:DTB:HCD1	3:A:702:DTB:HCT2	1.89	0.54
1:A:260:GLN:HA	1:A:263:LYS:HE3	1.88	0.54
1:A:114:LEU:HB3	1:A:151:VAL:HG13	1.90	0.53
1:A:42:LYS:NZ	1:A:46:GLU:OE2	2.34	0.53
1:A:381:ASP:OD1	1:A:384:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:CZ	3:A:702:DTB:HCR	2.43	0.53
1:A:534:GLU:HB3	1:A:540:ILE:HG13	1.91	0.52
1:A:579:ASP:HA	1:A:585:ALA:HB2	1.92	0.52
1:A:88:LEU:HD23	1:A:89:TYR:CE1	2.45	0.52
1:A:396:VAL:O	1:A:400:LEU:N	2.40	0.52
1:A:535:LEU:HD23	1:A:540:ILE:HB	1.92	0.52
1:A:279:LEU:HD12	1:A:630:LEU:HB2	1.90	0.52
1:A:161:TYR:OH	1:A:193:ASP:OD2	2.27	0.51
1:A:524:ASP:OD1	1:A:527:MET:HB2	2.11	0.51
1:A:506:ALA:O	1:A:510:ILE:HG12	2.10	0.50
1:A:236:ASN:N	1:A:240:LEU:O	2.45	0.49
1:A:420:LEU:H	1:A:421:GLY:CA	2.25	0.49
1:A:480:MET:HA	1:A:484:MET:HG3	1.93	0.49
1:A:89:TYR:O	1:A:91:ASN:N	2.46	0.49
1:A:451:VAL:HG12	1:A:452:PRO:HD3	1.85	0.49
1:A:578:GLY:HA2	1:A:581:HIS:CD2	2.47	0.49
1:A:464:VAL:O	1:A:464:VAL:HG22	2.13	0.48
1:A:262:ARG:HH12	1:A:281:GLU:HG3	1.77	0.48
1:A:337:LEU:HA	1:A:340:ILE:HG22	1.95	0.48
1:A:71:GLU:O	1:A:74:GLN:HB2	2.13	0.48
1:A:238:GLN:HG3	1:A:240:LEU:HD13	1.95	0.48
1:A:535:LEU:HD11	1:A:543:PRO:HD3	1.96	0.48
1:A:420:LEU:N	1:A:421:GLY:HA3	2.25	0.48
1:A:451:VAL:HG23	1:A:553:MET:HE1	1.96	0.47
1:A:441:MET:HG2	1:A:449:GLU:HA	1.96	0.47
1:A:338:TYR:CE1	1:A:394:GLY:HA3	2.49	0.47
1:A:442:ARG:HG3	1:A:443:LEU:H	1.79	0.47
1:A:192:GLN:HG2	1:A:198:THR:HG22	1.95	0.47
1:A:468:ALA:HB2	1:A:494:TRP:CD1	2.49	0.47
1:A:463:ASN:O	1:A:466:TYR:HB3	2.15	0.47
1:A:350:PRO:HB2	1:A:372:LEU:HD13	1.95	0.46
1:A:56:ASN:ND2	1:A:56:ASN:O	2.49	0.46
1:A:519:LEU:CD2	1:A:550:LEU:HD21	2.46	0.46
1:A:472:GLN:HB3	1:A:474:LEU:HD12	2.00	0.44
1:A:437:VAL:O	1:A:441:MET:N	2.45	0.44
1:A:535:LEU:CD2	1:A:542:GLY:HA2	2.48	0.44
1:A:625:GLY:HA3	1:A:626:ASP:HA	1.68	0.44
1:A:284:SER:OG	1:A:285:SER:N	2.51	0.44
1:A:40:GLN:O	1:A:44:ILE:HG12	2.18	0.44
1:A:92:ASN:OD1	1:A:129:ASN:ND2	2.50	0.44
1:A:218:LEU:O	1:A:221:SER:OG	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLN:HA	1:A:77:ALA:HB3	2.00	0.43
1:A:406:ILE:HD12	1:A:407:PHE:CD2	2.53	0.43
1:A:365:THR:CG2	1:A:367:LEU:HD12	2.43	0.43
1:A:307:LEU:HD22	1:A:597:VAL:HG11	2.01	0.43
1:A:462:CYS:O	1:A:465:MET:HG2	2.18	0.43
1:A:492:PHE:CG	1:A:572:LEU:HD22	2.53	0.43
3:A:702:DTB:CD	3:A:702:DTB:HCT2	2.47	0.43
1:A:354:ARG:HB3	1:A:368:GLN:HA	2.00	0.43
1:A:465:MET:HA	1:A:494:TRP:HE1	1.84	0.42
1:A:325:ARG:NE	1:A:471:PHE:O	2.52	0.42
1:A:469:ARG:NH1	1:A:595:GLN:HB3	2.34	0.42
1:A:190:ARG:HH12	1:A:229:LYS:HB3	1.83	0.42
1:A:190:ARG:NH1	1:A:229:LYS:HB3	2.34	0.42
1:A:589:ASP:O	1:A:593:ARG:HG3	2.20	0.42
1:A:406:ILE:CD1	1:A:407:PHE:CD2	3.03	0.42
1:A:296:VAL:HG23	1:A:297:THR:HG23	2.01	0.42
1:A:213:CYS:SG	1:A:253:VAL:HG12	2.60	0.41
1:A:427:ILE:HG23	1:A:459:LEU:HG	2.02	0.41
1:A:114:LEU:HA	1:A:150:SER:HB3	2.02	0.41
1:A:451:VAL:HG23	1:A:553:MET:HE3	2.01	0.41
1:A:497:ALA:O	1:A:501:LEU:HG	2.20	0.41
1:A:220:LEU:HD21	1:A:232:GLU:HG3	2.01	0.41
1:A:74:GLN:HE21	1:A:74:GLN:HB2	1.67	0.41
1:A:137:LEU:HA	1:A:137:LEU:HD13	1.93	0.41
1:A:244:LYS:HB2	1:A:244:LYS:HE3	1.83	0.41
1:A:289:GLN:NE2	1:A:289:GLN:O	2.54	0.41
1:A:381:ASP:O	1:A:384:ARG:HG3	2.21	0.41
1:A:461:TRP:CD1	1:A:502:GLY:HA2	2.56	0.41
1:A:338:TYR:HE1	1:A:394:GLY:HA3	1.86	0.41
1:A:448:GLY:O	1:A:451:VAL:HG12	2.21	0.41
1:A:190:ARG:HG2	1:A:190:ARG:H	1.73	0.40
1:A:620:ARG:NH2	1:A:626:ASP:OD2	2.54	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	598/668 (90%)	551 (92%)	41 (7%)	6 (1%)	18	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	481	ILE
1	A	71	GLU
1	A	377	VAL
1	A	374	GLU
1	A	355	ILE

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	518/580 (89%)	484 (93%)	34 (7%)	19	54

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	TRP
1	A	49	LEU
1	A	139	ARG
1	A	236	ASN
1	A	243	PHE
1	A	279	LEU
1	A	282	ILE
1	A	287	ASP
1	A	289	GLN
1	A	314	GLU
1	A	349	ARG

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Mol	Chain	Res	Type
1	A	355	ILE
1	A	366	LEU
1	A	368	GLN
1	A	373	GLN
1	A	374	GLU
1	A	382	ASP
1	A	384	ARG
1	A	399	LEU
1	A	441	MET
1	A	469	ARG
1	A	474	LEU
1	A	491	ARG
1	A	522	PHE
1	A	527	MET
1	A	539	ILE
1	A	586	HIS
1	A	591	LEU
1	A	605	ARG
1	A	609	ARG
1	A	621	GLU
1	A	622	TYR
1	A	627	ARG
1	A	631	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	206	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	12,15,15	0.65	0	12,19,19	1.15	0

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	-	-	0/6/20/20	0/1/1/1

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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	DTB	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	602/668 (90%)	0.36	43 (7%) 17 17	98, 129, 187, 248	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	576	MET	5.2
1	A	603	LEU	5.2
1	A	227	HIS	5.1
1	A	382	ASP	4.6
1	A	606	LYS	4.4
1	A	358	ARG	4.2
1	A	360	ASN	4.2
1	A	471	PHE	4.0
1	A	383	LEU	3.9
1	A	361	PRO	3.7
1	A	68	GLU	3.6
1	A	351	LEU	3.6
1	A	355	ILE	3.6
1	A	610	CYS	3.4
1	A	443	LEU	3.1
1	A	581	HIS	2.9
1	A	472	GLN	2.8
1	A	380	LYS	2.8
1	A	62	TYR	2.8
1	A	580	THR	2.7
1	A	228	LEU	2.7
1	A	137	LEU	2.7
1	A	612	TRP	2.6
1	A	611	LEU	2.6
1	A	608	PRO	2.6
1	A	607	LEU	2.5
1	A	141	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	142	SER	2.3
1	A	579	ASP	2.2
1	A	282	ILE	2.2
1	A	407	PHE	2.2
1	A	166	PRO	2.2
1	A	613	PRO	2.2
1	A	303	ALA	2.1
1	A	327	TYR	2.1
1	A	486	PHE	2.1
1	A	357	ASN	2.1
1	A	359	THR	2.1
1	A	248	VAL	2.1
1	A	582	TRP	2.1
1	A	538	THR	2.1
1	A	190	ARG	2.1
1	A	540	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	DTB	A	702	15/15	0.91	0.40	1.80	92,103,113,122	0
2	CA	A	701	1/1	0.88	0.76	-	111,111,111,111	1

6.5 Other polymers [i](#)

There are no such residues in this entry.