Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 05:57 PM EDT

PDB ID	:	6D7P
Title	:	Crystal Structure of Rat TRPV6*-Y466A
Authors	:	Singh, A.K.; Saotome, K.; McGoldrick, L.L.; Sobolevsky, A.I.
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 (i) 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 (1)) were used in the production of this report:

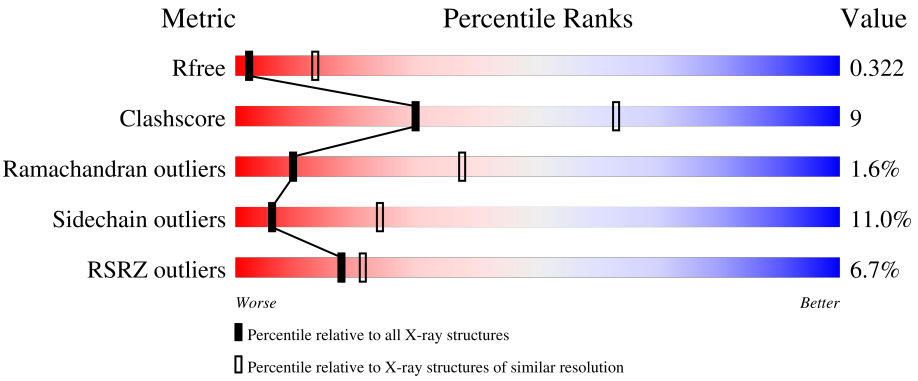
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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 <=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	6% 65% 22% · 9%

2 Entry composition (i)

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			

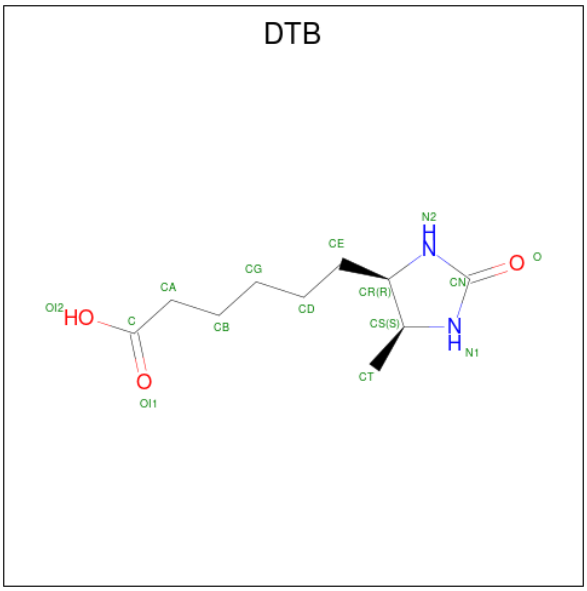
There are 7 discrepancies between the modelled and reference sequences:

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 (three-letter code: 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 (three-letter code: DTB) (formula: $C_{10}H_{18}N_2O_3$).



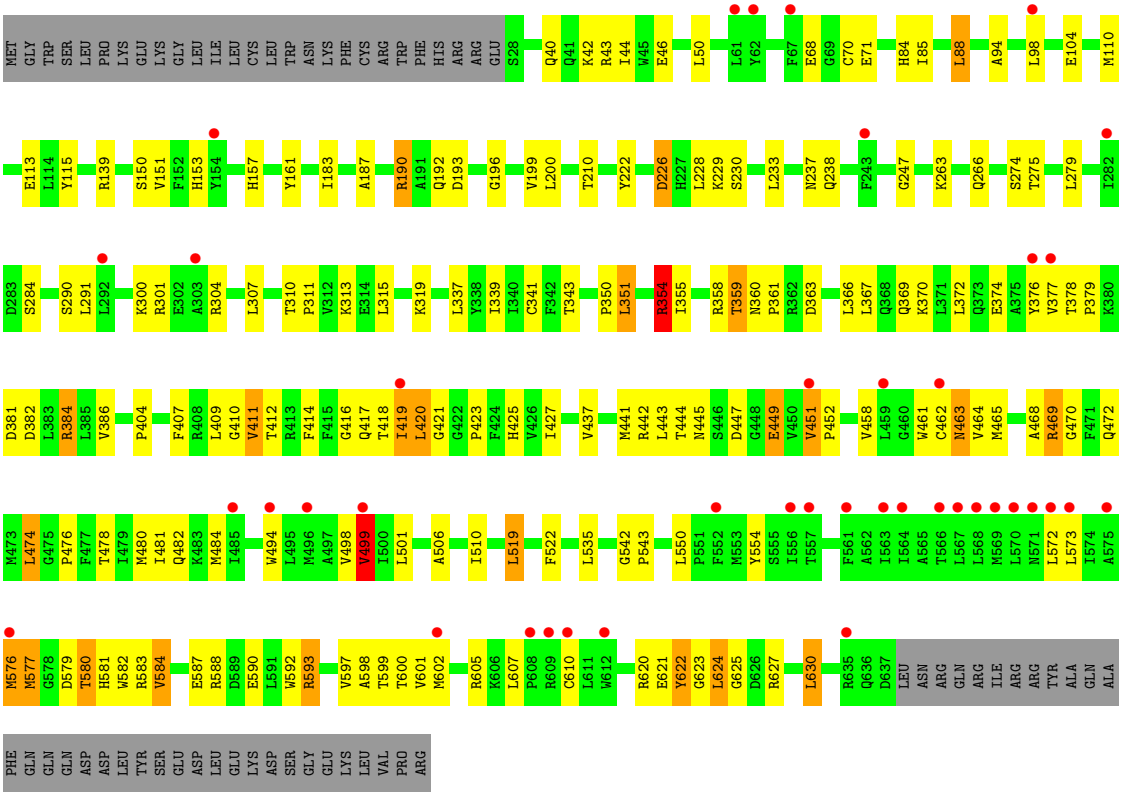
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	10	2	3	0	0

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

Chain A:



4 Data and refinement statistics (i)

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) 94.2 (116.49-3.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.295 , 0.310 0.305 , 0.322	Depositor DCC
R_{free} test set	831 reflections (4.78%)	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)	0.30 , 102.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.26	0/4957	0.47	1/6738 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	519	LEU	CA-CB-CG	5.85	128.75	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	4845	0	4866	92	0
2	A	2	0	0	0	0
3	A	15	0	17	1	0
All	All	4862	0	4883	92	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 9.

All (92) 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
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: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: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: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:484:MET:SD	1:A:576:MET:HE1	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:351:LEU:O	1:A:370:LYS:HA	2.17	0.44
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:469:ARG:HH11	1:A:599:THR:HG1	1.61	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:442:ARG:C	1:A:444:THR:H	2.23	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%)	9 37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	PRO
1	A	411	VAL
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 (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	520/583 (89%)	463 (89%)	57 (11%)	6 24

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	A	70	CYS
1	A	71	GLU
1	A	88	LEU
1	A	113	GLU
1	A	139	ARG
1	A	190	ARG
1	A	199	VAL
1	A	200	LEU
1	A	210	THR
1	A	226	ASP
1	A	228	LEU
1	A	263	LYS
1	A	275	THR
1	A	337	LEU
1	A	341	CYS
1	A	351	LEU
1	A	354	ARG
1	A	355	ILE
1	A	366	LEU
1	A	367	LEU
1	A	372	LEU
1	A	384	ARG
1	A	386	VAL
1	A	409	LEU
1	A	417	GLN
1	A	419	ILE
1	A	420	LEU
1	A	447	ASP
1	A	449	GLU

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Mol	Chain	Res	Type
1	A	451	VAL
1	A	458	VAL
1	A	463	ASN
1	A	469	ARG
1	A	472	GLN
1	A	474	LEU
1	A	481	ILE
1	A	499	VAL
1	A	501	LEU
1	A	519	LEU
1	A	522	PHE
1	A	550	LEU
1	A	572	LEU
1	A	573	LEU
1	A	576	MET
1	A	577	MET
1	A	579	ASP
1	A	580	THR
1	A	582	TRP
1	A	584	VAL
1	A	593	ARG
1	A	607	LEU
1	A	610	CYS
1	A	622	TYR
1	A	624	LEU
1	A	627	ARG
1	A	630	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	3.11	3 (20%)	16,19,19	2.82	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	8.17	1.48	1.35
3	A	703	DTB	CN-N1	7.94	1.48	1.35
3	A	703	DTB	O-CN	-2.15	1.18	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	703	DTB	CT-CS-N1	-6.77	103.63	111.70
3	A	703	DTB	CR-CS-N1	4.74	108.21	102.43
3	A	703	DTB	CS-CR-N2	4.42	107.70	102.17
3	A	703	DTB	CS-N1-CN	-3.73	108.29	112.42
3	A	703	DTB	CR-N2-CN	-3.52	107.88	112.46

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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	DTB	1	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, 95^{th} 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%)	0.37	41 (6%)	17	21	81, 123, 169, 188	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	609	ARG	5.7
1	A	496	MET	3.6
1	A	610	CYS	3.5
1	A	61	LEU	3.2
1	A	376	TYR	3.2
1	A	462	CYS	3.2
1	A	570	LEU	3.2
1	A	494	TRP	3.1
1	A	499	VAL	3.1
1	A	576	MET	3.0
1	A	62	TYR	2.9
1	A	485	ILE	2.8
1	A	557	THR	2.7
1	A	573	LEU	2.7
1	A	635	ARG	2.7
1	A	552	PHE	2.7
1	A	67	PHE	2.6
1	A	608	PRO	2.4
1	A	459	LEU	2.4
1	A	612	TRP	2.4
1	A	154	TYR	2.4
1	A	567	LEU	2.4
1	A	377	VAL	2.3
1	A	98	LEU	2.3
1	A	568	LEU	2.3
1	A	572	LEU	2.3
1	A	575	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	243	PHE	2.3
1	A	282	ILE	2.2
1	A	451	VAL	2.2
1	A	292	LEU	2.2
1	A	569	MET	2.2
1	A	556	ILE	2.2
1	A	563	ILE	2.1
1	A	561	PHE	2.1
1	A	419	ILE	2.0
1	A	303	ALA	2.0
1	A	602	MET	2.0
1	A	566	THR	2.0
1	A	571	ASN	2.0
1	A	564	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 monosaccharides 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, 95^{th} 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	0.35	0.08	132,132,132,132	1
3	DTB	A	703	15/15	0.87	0.33	118,118,118,118	0
2	CA	A	701	1/1	0.97	0.33	129,129,129,129	1

6.5 Other polymers (i)

There are no such residues in this entry.