Full wwPDB X-ray Structure Validation Report (i)

Jun 29, 2016 – 02:34 PM EDT

PDB ID	:	5IWT
Title	:	Structure of Transient Receptor Potential (TRP) channel TRPV6 in the presence of gadolinium
Authors	:	Saotome, K.; Singh, A.K.; Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on	:	2016-03-22
Resolution	:	3.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

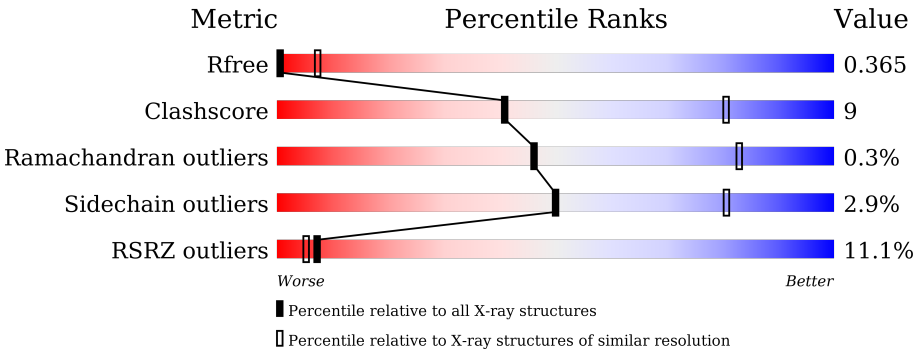
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 3.80 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 <=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	10% 71% 16% · 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DTB	A	703	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4759 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
			4742	3065	796	848	33			

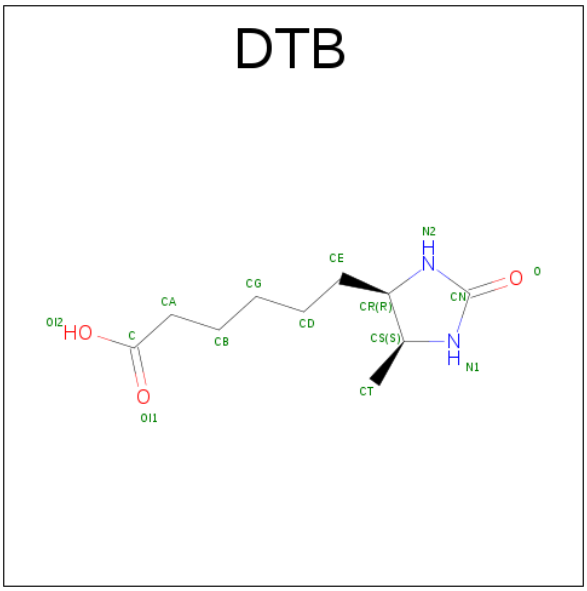
There are 7 discrepancies between the modelled and reference sequences:

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 GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Gd	0	0
			2	2		

- Molecule 3 is 6-(5-METHYL-2-OXO-IMIDAZOLIDIN-4-YL)-HEXANOIC ACID (three-letter code: DTB) (formula: $C_{10}H_{18}N_2O_3$).



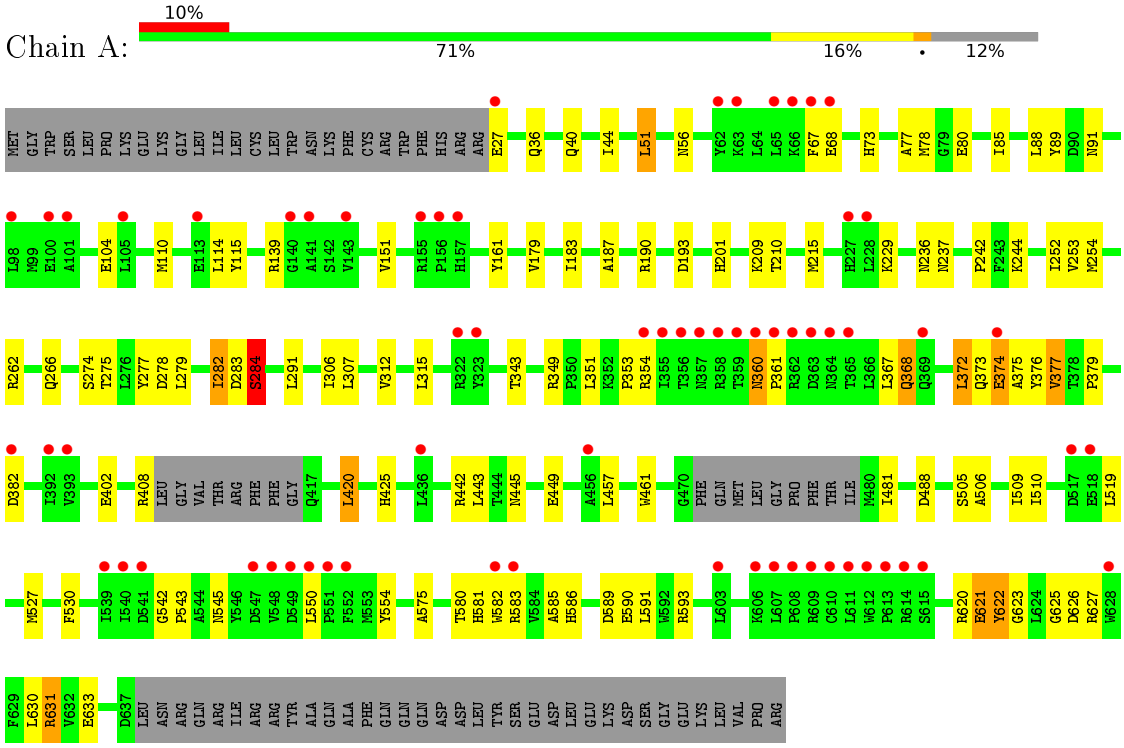
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	10	2	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	144.35Å 144.35Å 113.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 3.80 49.56 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.56-3.80) 99.2 (49.56-3.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.275 , 0.307 0.286 , 0.365	Depositor DCC
R_{free} test set	611 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	162.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 78.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	4759	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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, GD

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	0.39	1/4849 (0.0%)	0.63	11/6586 (0.2%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	SER	CB-OG	-7.13	1.32	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	284	SER	CB-CA-C	-13.46	84.52	110.10
1	A	351	LEU	N-CA-C	10.65	139.75	111.00
1	A	67	PHE	N-CA-C	-8.56	87.89	111.00
1	A	622	TYR	N-CA-C	7.88	132.28	111.00
1	A	622	TYR	CB-CA-C	-7.51	95.38	110.40
1	A	420	LEU	N-CA-C	-7.50	90.74	111.00
1	A	68	GLU	N-CA-C	-7.42	90.96	111.00
1	A	284	SER	N-CA-C	6.35	128.16	111.00
1	A	67	PHE	CB-CA-C	5.23	120.85	110.40
1	A	374	GLU	CB-CA-C	-5.22	99.95	110.40
1	A	351	LEU	CB-CA-C	-5.07	100.57	110.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	SER	Mainchain
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	4742	0	4762	80	3
2	A	2	0	0	0	0
3	A	15	0	17	4	0
All	All	4759	0	4779	82	3

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 (82) 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:590:GLU:HA	1:A:593:ARG:HB2	1.72	0.71
1:A:543:PRO:O	1:A:554:TYR:OH	2.06	0.68
1:A:78:MET:SD	1:A:115:TYR:HE2	2.17	0.67
1:A:527:MET:O	1:A:530:PHE:N	2.30	0.64
1:A:183:ILE:HD13	1:A:187:ALA:HB3	1.84	0.59
1:A:373:GLN:C	1:A:375:ALA:H	2.05	0.59
1:A:73:HIS:HE2	1:A:104:GLU:HG3	1.70	0.56
3:A:703:DTB:HCT2	3:A:703:DTB:HCD1	1.88	0.55
1:A:275:THR:HG23	1:A:277:TYR:CE2	2.42	0.55
1:A:377:VAL:O	1:A:377:VAL:HG23	2.05	0.54
1:A:115:TYR:CE1	3:A:703:DTB:HCR	2.43	0.54
1:A:78:MET:SD	1:A:115:TYR:CE2	3.02	0.53
1:A:402:GLU:OE2	1:A:425:HIS:ND1	2.42	0.52
1:A:585:ALA:O	1:A:589:ASP:HB2	2.09	0.52
1:A:519:LEU:HD13	1:A:545:ASN:HB2	1.91	0.51
1:A:89:TYR:N	1:A:89:TYR:CD1	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLU:C	1:A:376:TYR:H	2.13	0.51
1:A:372:LEU:HD13	1:A:375:ALA:CB	2.42	0.50
1:A:442:ARG:O	1:A:443:LEU:HB2	2.11	0.50
1:A:343:THR:HG21	1:A:461:TRP:HE1	1.75	0.50
1:A:40:GLN:HA	1:A:77:ALA:HB3	1.95	0.49
1:A:506:ALA:O	1:A:510:ILE:HG12	2.12	0.49
1:A:343:THR:HG22	1:A:457:LEU:HD22	1.95	0.49
1:A:481:ILE:HB	1:A:580:THR:HG22	1.94	0.48
1:A:626:ASP:O	1:A:626:ASP:CG	2.51	0.48
1:A:373:GLN:C	1:A:375:ALA:N	2.66	0.48
1:A:590:GLU:HG3	1:A:590:GLU:O	2.07	0.48
1:A:190:ARG:NH2	1:A:229:LYS:O	2.46	0.47
1:A:56:ASN:ND2	1:A:56:ASN:O	2.47	0.47
1:A:88:LEU:HD23	1:A:89:TYR:CE1	2.49	0.47
1:A:372:LEU:HB3	1:A:375:ALA:HB2	1.96	0.47
1:A:262:ARG:HB2	1:A:278:ASP:HB2	1.97	0.47
1:A:252:ILE:HD13	1:A:306:ILE:HD13	1.97	0.46
1:A:360:ASN:HB2	1:A:361:PRO:HD3	1.98	0.46
1:A:73:HIS:NE2	1:A:104:GLU:HG3	2.29	0.46
1:A:382:ASP:OD1	1:A:382:ASP:O	2.34	0.46
1:A:443:LEU:N	1:A:443:LEU:HD12	2.31	0.46
1:A:179:VAL:HG21	1:A:215:MET:SD	2.56	0.45
1:A:590:GLU:HG3	1:A:591:LEU:N	2.21	0.45
1:A:236:ASN:OD1	1:A:237:ASN:N	2.49	0.45
1:A:442:ARG:NH1	1:A:449:GLU:OE2	2.50	0.45
1:A:449:GLU:O	1:A:449:GLU:HG2	2.17	0.45
1:A:625:GLY:O	1:A:626:ASP:HB3	2.15	0.45
1:A:586:HIS:HA	1:A:589:ASP:HB3	2.00	0.44
1:A:114:LEU:O	1:A:151:VAL:HG22	2.18	0.44
1:A:254:MET:HE3	1:A:254:MET:HB3	1.82	0.43
1:A:376:TYR:O	1:A:377:VAL:C	2.56	0.43
1:A:201:HIS:CE1	1:A:242:PRO:HD3	2.53	0.43
1:A:620:ARG:O	1:A:621:GLU:C	2.57	0.43
3:A:703:DTB:CD	3:A:703:DTB:HCT2	2.48	0.43
1:A:279:LEU:HD22	1:A:630:LEU:HB2	2.01	0.42
1:A:266:GLN:OE1	1:A:274:SER:OG	2.32	0.42
1:A:307:LEU:C	1:A:307:LEU:HD12	2.39	0.42
1:A:488:ASP:HB3	1:A:575:ALA:HB1	2.02	0.42
1:A:51:LEU:O	1:A:51:LEU:HD12	2.20	0.42
1:A:543:PRO:HB2	1:A:554:TYR:CZ	2.55	0.42
1:A:80:GLU:HG3	1:A:85:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:TYR:O	1:A:91:ASN:N	2.48	0.42
1:A:283:ASP:OD1	1:A:284:SER:N	2.48	0.42
1:A:367:LEU:HD12	1:A:367:LEU:N	2.34	0.42
1:A:110:MET:HB2	1:A:115:TYR:O	2.21	0.41
1:A:179:VAL:O	1:A:183:ILE:HG12	2.21	0.41
1:A:542:GLY:O	1:A:543:PRO:C	2.58	0.41
1:A:582:TRP:CG	1:A:583:ARG:N	2.88	0.41
1:A:210:THR:HA	1:A:253:VAL:HG11	2.03	0.41
1:A:40:GLN:O	1:A:44:ILE:HG12	2.21	0.41
1:A:354:ARG:HB2	1:A:368:GLN:HA	2.03	0.41
1:A:621:GLU:H	1:A:623:GLY:H	1.69	0.41
1:A:27:GLU:O	1:A:27:GLU:HG2	2.22	0.41
1:A:586:HIS:O	1:A:589:ASP:HB3	2.20	0.41
1:A:114:LEU:HB2	1:A:115:TYR:CE2	2.57	0.40
1:A:161:TYR:OH	1:A:193:ASP:OD2	2.31	0.40
1:A:244:LYS:HB2	1:A:244:LYS:HE3	1.79	0.40
1:A:279:LEU:HD21	1:A:315:LEU:HD13	2.03	0.40
1:A:373:GLN:HB2	1:A:445:ASN:HD21	1.86	0.40
1:A:505:SER:O	1:A:509:ILE:HG12	2.21	0.40
1:A:282:ILE:HG21	1:A:312:VAL:HG22	2.04	0.40
1:A:360:ASN:N	1:A:360:ASN:OD1	2.54	0.40
1:A:40:GLN:HE22	3:A:703:DTB:HN1	1.68	0.40
1:A:209:LYS:HB3	1:A:253:VAL:HB	2.04	0.40
1:A:36:GLN:O	1:A:40:GLN:N	2.52	0.40
1:A:631:ARG:NH2	1:A:633:GLU:OE2	2.54	0.40

All (3) 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:581:HIS:ND1	1:A:581:HIS:CE1[3_555]	1.59	0.61
1:A:581:HIS:CE1	1:A:581:HIS:CE1[3_555]	1.79	0.41
1:A:581:HIS:O	1:A:581:HIS:NE2[3_555]	2.03	0.17

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	588/672 (88%)	544 (92%)	42 (7%)	2 (0%)	46 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	PRO
1	A	377	VAL

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	511/584 (88%)	496 (97%)	15 (3%)	50 81

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	139	ARG
1	A	282	ILE
1	A	291	LEU
1	A	349	ARG
1	A	353	PRO
1	A	360	ASN
1	A	368	GLN
1	A	372	LEU
1	A	408	ARG
1	A	420	LEU
1	A	550	LEU
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	445	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

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	-	12,15,15	0.72	0	14,19,19	1.12	1 (7%)

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	-	-	0/6/20/20	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(^{o})	Ideal(^{o})
3	A	703	DTB	CR-N2-CN	2.06	114.06	112.49

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	703	DTB	4	0

5.7 Other polymers

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, 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	594/672 (88%)	0.39	66 (11%) 7 5	98, 137, 214, 256	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	ASN	9.7
1	A	359	THR	9.4
1	A	364	ASN	7.5
1	A	549	ASP	6.0
1	A	361	PRO	6.0
1	A	358	ARG	4.8
1	A	365	THR	4.8
1	A	62	TYR	4.7
1	A	606	LYS	4.3
1	A	551	PRO	4.2
1	A	354	ARG	4.2
1	A	68	GLU	4.2
1	A	67	PHE	4.1
1	A	552	PHE	4.0
1	A	363	ASP	3.8
1	A	369	GLN	3.6
1	A	393	VAL	3.6
1	A	612	TRP	3.4
1	A	157	HIS	3.2
1	A	609	ARG	3.2
1	A	65	LEU	3.2
1	A	436	LEU	3.2
1	A	362	ARG	3.1
1	A	548	VAL	3.1
1	A	66	LYS	3.1
1	A	227	HIS	3.0
1	A	611	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	615	SER	2.8
1	A	357	ASN	2.8
1	A	228	LEU	2.8
1	A	608	PRO	2.7
1	A	105	LEU	2.7
1	A	322	ARG	2.7
1	A	550	LEU	2.6
1	A	610	CYS	2.6
1	A	607	LEU	2.5
1	A	603	LEU	2.5
1	A	582	TRP	2.5
1	A	355	ILE	2.5
1	A	614	ARG	2.5
1	A	323	TYR	2.5
1	A	374	GLU	2.5
1	A	517	ASP	2.5
1	A	583	ARG	2.4
1	A	613	PRO	2.4
1	A	100	GLU	2.3
1	A	456	ALA	2.3
1	A	540	ILE	2.3
1	A	628	TRP	2.3
1	A	156	PRO	2.3
1	A	541	ASP	2.3
1	A	539	ILE	2.2
1	A	113	GLU	2.2
1	A	140	GLY	2.2
1	A	143	VAL	2.2
1	A	98	LEU	2.2
1	A	101	ALA	2.2
1	A	141	ALA	2.1
1	A	382	ASP	2.1
1	A	63	LYS	2.1
1	A	518	GLU	2.1
1	A	27	GLU	2.1
1	A	356	THR	2.0
1	A	547	ASP	2.0
1	A	155	ARG	2.0
1	A	392	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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	DTB	A	703	15/15	0.83	0.46	1.88	139,149,165,171	0
2	GD	A	702	1/1	0.65	0.22	-	271,271,271,271	0
2	GD	A	701	1/1	0.97	0.37	-	142,142,142,142	1

6.5 Other polymers (i)

There are no such residues in this entry.