



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:12 am BST

PDB ID : 6D7O
Title : Crystal Structure of Rat TRPV6* in complex with 2-Aminoethoxydiphenyl borate (2-APB)
Authors : Singh, A.K.; Saotome, K.; McGoldrick, L.L.; Sobolevsky, A.I.
Deposited on : 2018-04-25
Resolution : 3.45 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

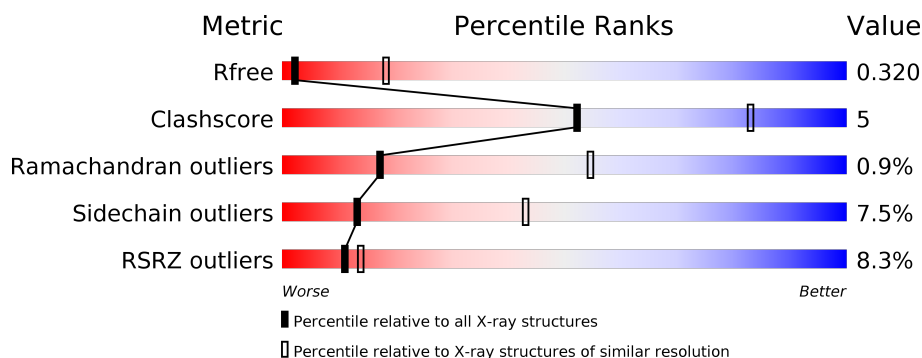
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 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	<div> <div>7%</div> <div>71%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>

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
4	DTB	A	703	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4758 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	592	Total	C	N	O	S	0	0	0
			4725	3059	791	841	34			

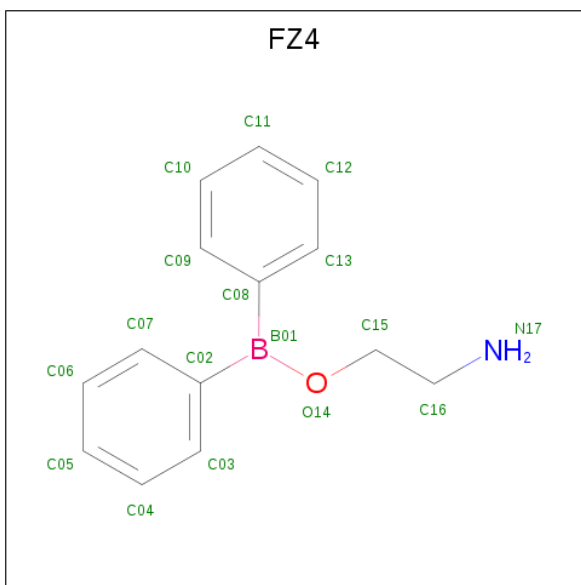
There are 6 discrepancies between the modelled and reference sequences:

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	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).

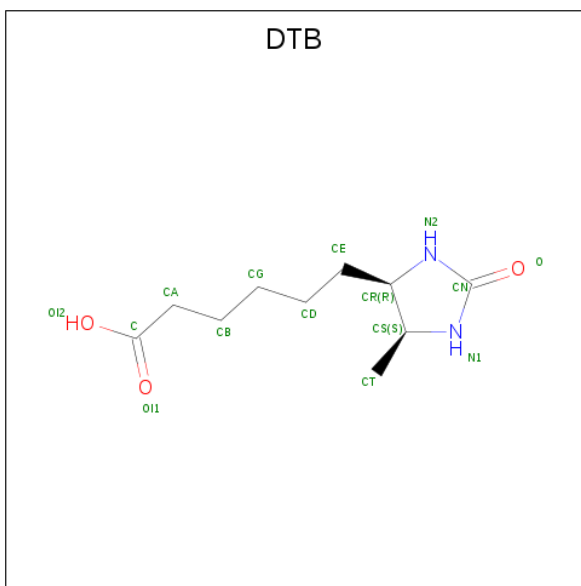
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2-aminoethyl diphenylborinate (three-letter code: FZ4) (formula: C₁₄H₁₆BNO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	B	C	N	O	0	0
			17	1	14	1	1		

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

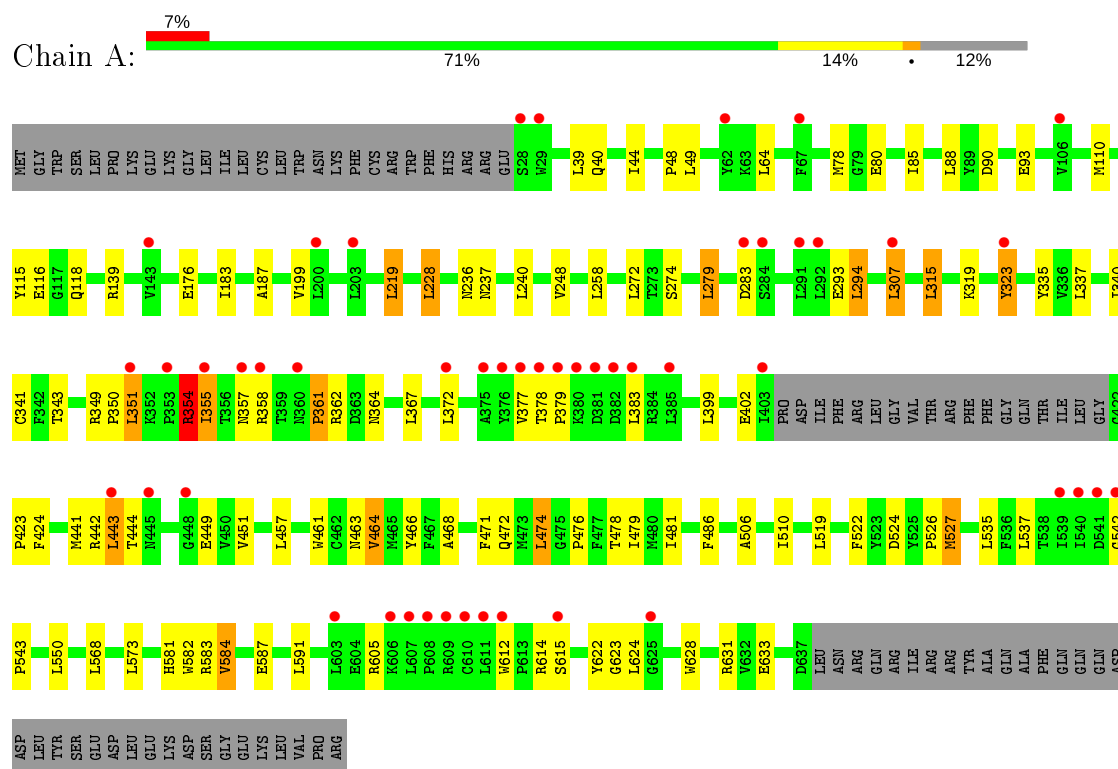


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	10	2	3		

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	145.38 Å 145.38 Å 116.16 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.01 – 3.45 47.00 – 3.41	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.01-3.45) 95.0 (47.00-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 3.40 Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.285 , 0.316 0.285 , 0.320	Depositor DCC
R_{free} test set	833 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	143.2	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 94.3	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	4758	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, FZ4

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	0/4833	0.50	7/6564 (0.1%)

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	323	TYR	CB-CA-C	-7.95	94.50	110.40
1	A	307	LEU	CA-CB-CG	7.43	132.40	115.30
1	A	354	ARG	N-CA-C	7.05	130.03	111.00
1	A	354	ARG	O-C-N	-6.29	112.63	122.70
1	A	472	GLN	N-CA-CB	-5.53	100.64	110.60
1	A	355	ILE	N-CA-C	5.41	125.61	111.00
1	A	351	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	ARG	Mainchain

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	4725	0	4748	52	0
2	A	1	0	0	0	0
3	A	17	0	0	0	0
4	A	15	0	15	1	0
All	All	4758	0	4763	52	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 5.

All (52) 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:323:TYR:O	1:A:612:TRP:CZ3	2.11	1.03
1:A:581:HIS:O	1:A:584:VAL:HG23	1.71	0.90
1:A:323:TYR:O	1:A:612:TRP:HZ3	1.70	0.71
1:A:183:ILE:HD13	1:A:187:ALA:HB3	1.82	0.62
1:A:349:ARG:HB2	1:A:350:PRO:HD2	1.84	0.58
1:A:115:TYR:HE1	4:A:703:DTB:HCG1	1.68	0.58
1:A:519:LEU:HD21	1:A:543:PRO:HB3	1.84	0.58
1:A:524:ASP:HB2	1:A:527:MET:HB2	1.87	0.57
1:A:354:ARG:O	1:A:354:ARG:HG2	2.05	0.56
1:A:535:LEU:HD11	1:A:542:GLY:HA2	1.88	0.56
1:A:506:ALA:O	1:A:510:ILE:HG12	2.07	0.54
1:A:279:LEU:HD22	1:A:283:ASP:HB2	1.89	0.53
1:A:524:ASP:HB3	1:A:526:PRO:HD2	1.90	0.53
1:A:335:TYR:HD2	1:A:464:VAL:HG23	1.74	0.52
1:A:323:TYR:O	1:A:612:TRP:CE3	2.62	0.50
1:A:315:LEU:HD22	1:A:319:LYS:HD2	1.94	0.49
1:A:236:ASN:OD1	1:A:237:ASN:N	2.45	0.49
1:A:357:ASN:O	1:A:358:ARG:HD3	2.13	0.48
1:A:350:PRO:HB3	1:A:372:LEU:HB2	1.96	0.48
1:A:293:GLU:OE2	1:A:605:ARG:NH2	2.47	0.48
1:A:248:VAL:HG22	1:A:294:LEU:HB3	1.97	0.47
1:A:378:THR:N	1:A:379:PRO:HD2	2.30	0.47
1:A:476:PRO:HA	1:A:479:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HD21	1:A:615:SER:HB3	1.99	0.45
1:A:583:ARG:O	1:A:587:GLU:N	2.42	0.45
1:A:357:ASN:O	1:A:358:ARG:CD	2.65	0.44
1:A:423:PRO:HB3	1:A:486:PHE:CE2	2.52	0.44
1:A:478:THR:HA	1:A:481:ILE:HG22	2.00	0.44
1:A:442:ARG:O	1:A:443:LEU:HB2	2.17	0.44
1:A:424:PHE:CG	1:A:466:TYR:HB2	2.52	0.43
1:A:110:MET:HG3	1:A:118:GLN:HB3	1.99	0.43
1:A:461:TRP:O	1:A:464:VAL:HG12	2.19	0.43
1:A:48:PRO:HB2	1:A:64:LEU:HD21	2.01	0.43
1:A:80:GLU:HG3	1:A:85:ILE:HD11	2.01	0.43
1:A:343:THR:HG21	1:A:461:TRP:HE1	1.84	0.42
1:A:442:ARG:HG3	1:A:443:LEU:HD13	2.01	0.42
1:A:199:VAL:HG11	1:A:219:LEU:HD22	2.01	0.42
1:A:361:PRO:HB2	1:A:362:ARG:H	1.73	0.42
1:A:240:LEU:HA	1:A:240:LEU:HD12	1.86	0.42
1:A:471:PHE:HD2	1:A:474:LEU:HD11	1.84	0.42
1:A:622:TYR:O	1:A:624:LEU:N	2.50	0.42
1:A:442:ARG:C	1:A:444:THR:H	2.24	0.41
1:A:581:HIS:O	1:A:584:VAL:CG2	2.57	0.41
1:A:274:SER:HA	1:A:633:GLU:HA	2.02	0.41
1:A:582:TRP:CD1	1:A:582:TRP:N	2.89	0.41
1:A:614:ARG:HD3	1:A:628:TRP:CE2	2.56	0.41
1:A:40:GLN:O	1:A:44:ILE:HG12	2.21	0.41
1:A:93:GLU:N	1:A:93:GLU:OE1	2.53	0.41
1:A:463:ASN:O	1:A:466:TYR:HB3	2.21	0.40
1:A:228:LEU:HG	1:A:228:LEU:H	1.62	0.40
1:A:337:LEU:HA	1:A:340:ILE:HG22	2.03	0.40
1:A:468:ALA:HB1	1:A:474:LEU:HD13	2.03	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	586/672 (87%)	528 (90%)	53 (9%)	5 (1%)	17	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	PRO
1	A	355	ILE
1	A	377	VAL
1	A	116	GLU
1	A	623	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	508/584 (87%)	470 (92%)	38 (8%)	13	43

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	49	LEU
1	A	78	MET
1	A	88	LEU
1	A	90	ASP
1	A	139	ARG
1	A	176	GLU
1	A	219	LEU
1	A	228	LEU
1	A	258	LEU
1	A	272	LEU
1	A	279	LEU
1	A	294	LEU
1	A	307	LEU
1	A	315	LEU
1	A	341	CYS

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Mol	Chain	Res	Type
1	A	351	LEU
1	A	364	ASN
1	A	367	LEU
1	A	383	LEU
1	A	399	LEU
1	A	402	GLU
1	A	441	MET
1	A	443	LEU
1	A	449	GLU
1	A	451	VAL
1	A	457	LEU
1	A	464	VAL
1	A	474	LEU
1	A	522	PHE
1	A	527	MET
1	A	537	LEU
1	A	550	LEU
1	A	568	LEU
1	A	573	LEU
1	A	584	VAL
1	A	591	LEU
1	A	631	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	581	HIS

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, 1 is monoatomic - leaving 2 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$
4	DTB	A	703	-	12,15,15	5.14	4 (33%)	12,19,19	4.29	5 (41%)
3	FZ4	A	702	-	16,18,18	0.49	0	17,22,22	1.17	2 (11%)

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
4	DTB	A	703	-	2/2/4/6	3/6/20/20	0/1/1/1
3	FZ4	A	702	-	-	2/12/12/12	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	DTB	CS-N1	-12.06	1.32	1.46
4	A	703	DTB	CR-N2	-8.90	1.32	1.46
4	A	703	DTB	O-CN	8.08	1.40	1.23
4	A	703	DTB	CS-CR	-4.60	1.39	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	DTB	CT-CS-N1	12.55	126.64	111.70
4	A	703	DTB	CS-N1-CN	-4.14	107.84	112.42
4	A	703	DTB	CS-CR-N2	3.95	107.11	102.17
4	A	703	DTB	CR-CS-N1	3.79	107.05	102.43
4	A	703	DTB	CR-N2-CN	-3.50	107.90	112.46
3	A	702	FZ4	C07-C02-C03	2.54	119.72	116.88
3	A	702	FZ4	C13-C08-C09	2.30	119.45	116.88

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	703	DTB	CS
4	A	703	DTB	CR

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	DTB	CD-CE-CR-N2
3	A	702	FZ4	C02-B01-O14-C15
3	A	702	FZ4	C08-B01-O14-C15
4	A	703	DTB	CG-CD-CE-CR
4	A	703	DTB	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	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, 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	592/672 (88%)	0.40	49 (8%) 11 14	114, 136, 177, 203	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	ASN	4.7
1	A	357	ASN	4.5
1	A	382	ASP	4.5
1	A	607	LEU	4.5
1	A	606	LYS	4.5
1	A	380	LYS	4.3
1	A	608	PRO	4.2
1	A	355	ILE	4.2
1	A	379	PRO	4.1
1	A	284	SER	4.0
1	A	610	CYS	3.9
1	A	443	LEU	3.8
1	A	28	SER	3.7
1	A	609	ARG	3.5
1	A	541	ASP	3.2
1	A	292	LEU	3.0
1	A	540	ILE	2.9
1	A	376	TYR	2.8
1	A	403	ILE	2.8
1	A	378	THR	2.8
1	A	539	ILE	2.7
1	A	377	VAL	2.7
1	A	143	VAL	2.7
1	A	283	ASP	2.6
1	A	615	SER	2.6
1	A	383	LEU	2.6
1	A	291	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	372	LEU	2.5
1	A	323	TYR	2.5
1	A	625	GLY	2.4
1	A	307	LEU	2.4
1	A	351	LEU	2.4
1	A	445	ASN	2.3
1	A	200	LEU	2.3
1	A	358	ARG	2.3
1	A	62	TYR	2.2
1	A	67	PHE	2.2
1	A	611	LEU	2.2
1	A	542	GLY	2.2
1	A	603	LEU	2.2
1	A	106	VAL	2.2
1	A	612	TRP	2.1
1	A	385	LEU	2.1
1	A	29	TRP	2.1
1	A	448	GLY	2.1
1	A	353	PRO	2.1
1	A	375	ALA	2.1
1	A	381	ASP	2.1
1	A	203	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 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. 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
3	FZ4	A	702	17/17	0.78	0.23	144,148,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DTB	A	703	15/15	0.85	0.53	110,122,140,140	0
2	CA	A	701	1/1	0.99	0.62	140,140,140,140	1

6.5 Other polymers [i](#)

There are no such residues in this entry.