Full wwPDB X-ray Structure Validation Report (i)

Jun 29, 2022 – 02:03 PM JST

PDB ID	:	7Y6E
Title	:	Crystal structure of sDscam FNIII23 domains, isoform Beta2v6
Deposited on	:	2022-06-20
Resolution	:	3.05 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

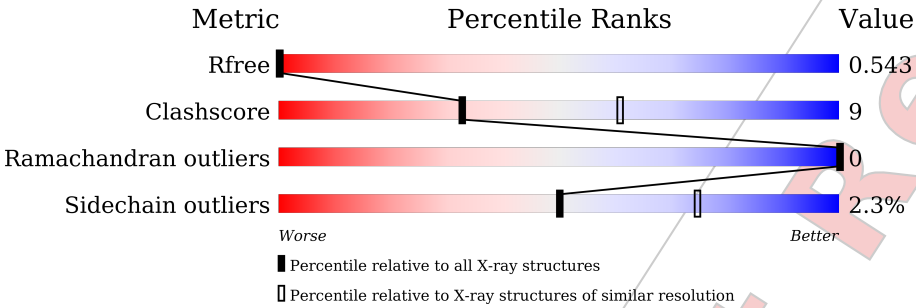
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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)

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%

Mol	Chain	Length	Quality of chain
1	D	202	77% 20% ••

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2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3040 atoms, of which 1483 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 Down Syndrome Cell Adhesion Molecules.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	D	199	3040	995	1483	267	293	2	0	0	0

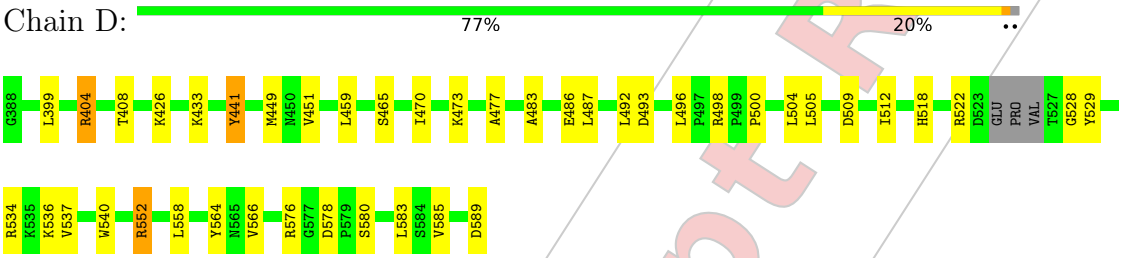
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3 Residue-property plots

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. 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. 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: Down Syndrome Cell Adhesion Molecules

Chain D:



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4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	307.02Å 56.22Å 94.84Å 90.00° 105.38° 90.00°	Depositor
Resolution (Å)	48.85 – 3.05 48.85 – 3.03	Depositor EDS
% Data completeness (in resolution range)	84.3 (48.85-3.05) 84.3 (48.85-3.03)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.12	Depositor
R, R_{free}	0.233 , 0.287 0.532 , 0.543	Depositor DCC
R_{free} test set	1373 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å^2)	61.7	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 5.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.39	EDS
Total number of atoms	3040	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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.

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5 Model quality

5.1 Standard geometry

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	D	0.53	0/1601	0.68	0/2182

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	D	1557	1483	1542	27	1
All	All	1557	1483	1542	27	1

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 (27) 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:D:465:SER:OG	1:D:493:ASP:OD1	1.89	0.90
1:D:505:LEU:HD12	1:D:552:ARG:HH12	1.55	0.69
1:D:404:ARG:NH1	1:D:578:ASP:OD1	2.26	0.67
1:D:505:LEU:HD12	1:D:552:ARG:NH1	2.13	0.63
1:D:558:LEU:HD22	1:D:564:TYR:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:ARG:NH1	1:D:552:ARG:HG2	2.22	0.53
1:D:512:ILE:HD13	1:D:585:VAL:HG13	1.92	0.52
1:D:449:MET:O	1:D:451:VAL:HG23	2.12	0.50
1:D:504:LEU:O	1:D:505:LEU:HD23	2.12	0.49
1:D:492:LEU:HD13	1:D:496:LEU:HD21	1.93	0.49
1:D:433:LYS:HG2	1:D:441:TYR:CE1	2.47	0.49
1:D:536:LYS:HG3	1:D:537:VAL:HG23	1.95	0.48
1:D:552:ARG:HG2	1:D:552:ARG:HH11	1.77	0.47
1:D:500:PRO:O	1:D:580:SER:CB	2.62	0.47
1:D:399:LEU:HD13	1:D:487:LEU:HD12	1.96	0.47
1:D:470:ILE:O	1:D:486:GLU:HA	2.15	0.47
1:D:509:ASP:HB3	1:D:589:ASP:OD1	2.14	0.47
1:D:500:PRO:O	1:D:580:SER:HB2	2.16	0.45
1:D:504:LEU:HG	1:D:583:LEU:HD21	1.98	0.44
1:D:408:THR:HA	1:D:459:LEU:O	2.16	0.44
1:D:534:ARG:HB3	1:D:540:TRP:HA	1.99	0.44
1:D:498:ARG:O	1:D:518:HIS:NE2	2.52	0.42
1:D:566:VAL:HG12	1:D:583:LEU:HB3	2.01	0.42
1:D:449:MET:O	1:D:451:VAL:N	2.53	0.42
1:D:473:LYS:HE2	1:D:483:ALA:HB2	2.00	0.42
1:D:528:GLY:C	1:D:529:TYR:HD2	2.23	0.42
1:D:426:LYS:HE3	1:D:477:ALA:HB2	2.03	0.41

All (1) 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:D:537:VAL:O	1:D:576:ARG:NH2[2_556]	2.14	0.06

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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	195/202 (96%)	177 (91%)	18 (9%)	0	100 100

There are no Ramachandran outliers to report.

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	D	171/174 (98%)	167 (98%)	4 (2%)	50 75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	404	ARG
1	D	441	TYR
1	D	522	ARG
1	D	552	ARG

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

Mol	Chain	Res	Type
1	D	542	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.

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5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

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6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.

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