



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:47 pm GMT

PDB ID : 3S9G
Title : Structure of human Hexim1 (delta stammer) coiled coil domain
Authors : Bigalke, J.M.; Blankenfeldt, W.; Geyer, M.
Deposited on : 2011-06-01
Resolution : 2.10 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

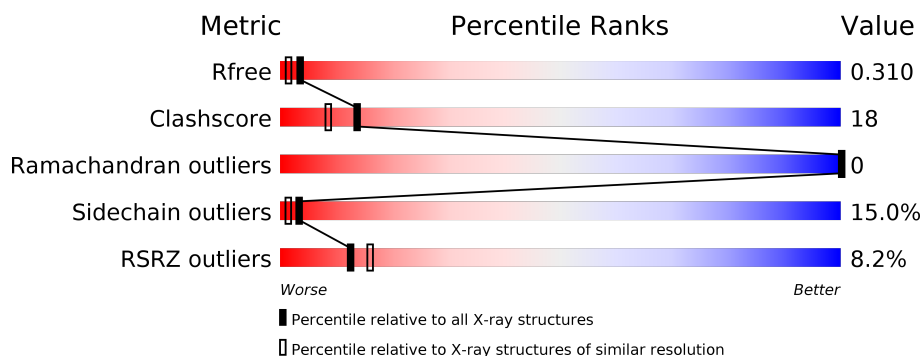
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	104	<div> <div>8%</div> <div> <div></div> <div>55%</div> <div>22%</div> <div>•</div> <div>21%</div> </div> </div>
1	B	104	<div> <div>5%</div> <div> <div></div> <div>45%</div> <div>21%</div> <div>6%</div> <div>•</div> <div>27%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1321 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 Protein HEXIM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	S	0	0	0
			648	395	115	136	2			
1	B	76	Total	C	N	O	S	0	0	0
			622	380	116	124	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	GLY	-	EXPRESSION TAG	UNP O94992
A	254	ALA	-	EXPRESSION TAG	UNP O94992
A	297	SER	CYS	ENGINEERED MUTATION	UNP O94992
A	?	-	GLY	DELETION	UNP O94992
A	?	-	GLY	DELETION	UNP O94992
A	?	-	ASP	DELETION	UNP O94992
B	253	GLY	-	EXPRESSION TAG	UNP O94992
B	254	ALA	-	EXPRESSION TAG	UNP O94992
B	297	SER	CYS	ENGINEERED MUTATION	UNP O94992
B	?	-	GLY	DELETION	UNP O94992
B	?	-	GLY	DELETION	UNP O94992
B	?	-	ASP	DELETION	UNP O94992

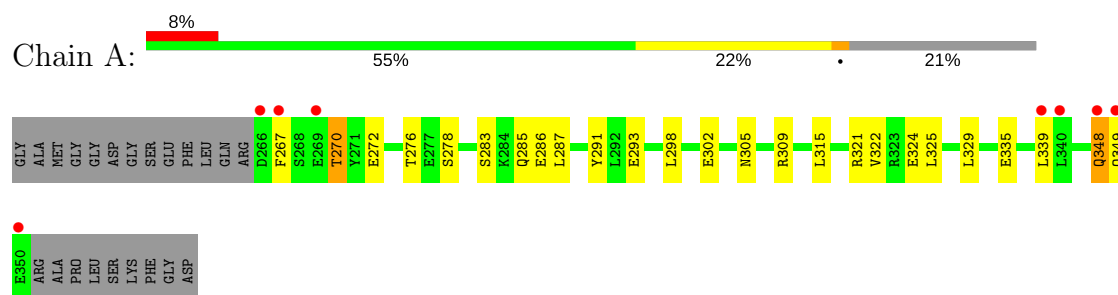
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		
2	B	34	Total	O	0	0
			34	34		

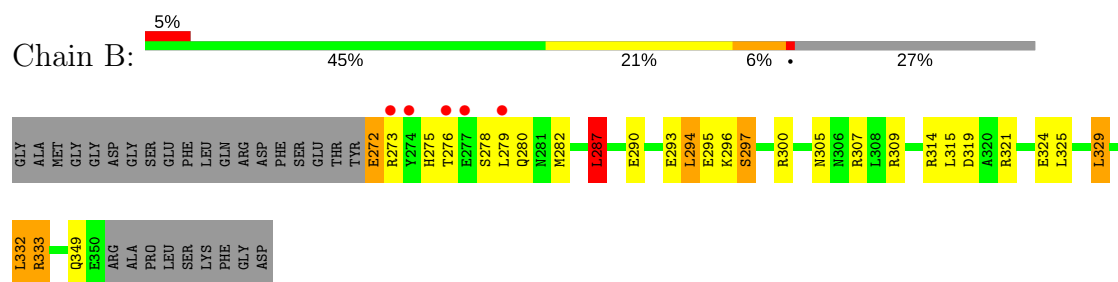
3 Residue-property plots [i](#)

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: Protein HEXIM1



• Molecule 1: Protein HEXIM1



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	70.77Å 70.77Å 90.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.50 – 2.10 35.38 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.50-2.10) 100.0 (35.38-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.236 , 0.296 0.249 , 0.310	Depositor DCC
R_{free} test set	629 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1321	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.84	0/651	0.95	0/876
1	B	1.15	3/624 (0.5%)	1.18	4/835 (0.5%)
All	All	1.01	3/1275 (0.2%)	1.07	4/1711 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	GLU	CD-OE2	-6.16	1.18	1.25
1	B	297	SER	CB-OG	-5.61	1.34	1.42
1	B	287	LEU	CA-CB	-5.25	1.41	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	B	287	LEU	CB-CA-C	-6.43	97.98	110.20
1	B	296	LYS	CD-CE-NZ	5.15	123.54	111.70
1	B	333	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	648	0	600	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	622	0	608	34	0
2	A	17	0	0	1	0
2	B	34	0	0	4	0
All	All	1321	0	1208	44	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 18.

All (44) 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:B:273:ARG:HA	1:B:276:THR:HG23	1.27	1.15
1:B:273:ARG:CA	1:B:276:THR:HG23	1.94	0.97
1:B:272:GLU:HG2	1:B:273:ARG:N	1.86	0.90
1:B:294:LEU:O	1:B:294:LEU:HD23	1.80	0.80
1:B:297:SER:HB3	1:B:300:ARG:NH2	1.96	0.80
1:B:287:LEU:HD12	1:B:287:LEU:O	1.86	0.75
1:A:267:PHE:CB	1:A:270:THR:HG23	2.20	0.72
1:B:294:LEU:CD2	1:B:294:LEU:C	2.58	0.71
1:B:294:LEU:HD23	1:B:294:LEU:C	2.09	0.70
1:B:309:ARG:NE	2:B:36:HOH:O	2.08	0.69
1:B:276:THR:HA	1:B:280:GLN:HE22	1.57	0.68
1:B:273:ARG:CB	1:B:276:THR:HG23	2.27	0.64
1:B:309:ARG:NH2	2:B:36:HOH:O	2.19	0.63
1:B:278:SER:O	1:B:282:MET:HE3	1.99	0.63
1:B:294:LEU:O	1:B:294:LEU:CD2	2.48	0.61
1:A:315:LEU:O	1:A:322:VAL:HG23	2.00	0.60
1:B:280:GLN:OE1	2:B:48:HOH:O	2.17	0.60
1:B:272:GLU:HG2	1:B:273:ARG:H	1.64	0.60
1:A:309:ARG:NH1	2:A:17:HOH:O	2.33	0.57
1:A:291:TYR:CE2	1:B:279:LEU:HD21	2.40	0.56
1:B:276:THR:O	1:B:280:GLN:CD	2.44	0.56
1:A:321:ARG:NE	1:A:325:LEU:HD11	2.21	0.55
1:A:315:LEU:HD21	1:B:319:ASP:OD1	2.07	0.55
1:A:272:GLU:O	1:A:276:THR:HG23	2.08	0.54
1:A:302:GLU:O	1:A:305:ASN:HB3	2.07	0.54
1:B:273:ARG:HA	1:B:276:THR:CG2	2.20	0.54
1:B:276:THR:O	1:B:280:GLN:HB2	2.08	0.52
1:B:278:SER:O	1:B:282:MET:CE	2.58	0.51
1:A:315:LEU:CD2	1:B:319:ASP:OD1	2.60	0.50
1:B:315:LEU:O	1:B:321:ARG:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:THR:HA	1:B:280:GLN:NE2	2.24	0.49
1:A:348:GLN:HG2	1:A:349:GLN:N	2.28	0.49
1:A:329:LEU:HD12	1:B:325:LEU:HD22	1.95	0.47
1:B:275:HIS:O	1:B:276:THR:C	2.53	0.47
1:A:329:LEU:CD2	1:B:332:LEU:HD13	2.46	0.46
1:B:273:ARG:CB	1:B:276:THR:CG2	2.93	0.46
1:B:294:LEU:HD22	1:B:294:LEU:C	2.37	0.43
1:A:267:PHE:CB	1:A:270:THR:CG2	2.94	0.43
1:B:272:GLU:CG	1:B:273:ARG:N	2.67	0.43
1:A:283:SER:OG	1:A:286:GLU:HG3	2.20	0.42
1:B:329:LEU:HD13	1:B:333:ARG:NH1	2.35	0.42
1:A:321:ARG:HG3	1:A:325:LEU:HD12	2.01	0.42
1:A:305:ASN:CA	1:B:305:ASN:HD21	2.32	0.42
1:B:295:GLU:HG2	2:B:38:HOH:O	2.21	0.41

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	80/104 (77%)	72 (90%)	8 (10%)	0	100	100
1	B	74/104 (71%)	69 (93%)	5 (7%)	0	100	100
All	All	154/208 (74%)	141 (92%)	13 (8%)	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	A	67/95 (70%)	57 (85%)	10 (15%)	3	1
1	B	66/95 (70%)	56 (85%)	10 (15%)	3	1
All	All	133/190 (70%)	113 (85%)	20 (15%)	3	1

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	THR
1	A	278	SER
1	A	285	GLN
1	A	287	LEU
1	A	293	GLU
1	A	298	LEU
1	A	324	GLU
1	A	335	GLU
1	A	339	LEU
1	A	348	GLN
1	B	272	GLU
1	B	287	LEU
1	B	290	GLU
1	B	294	LEU
1	B	307	ARG
1	B	314	ARG
1	B	324	GLU
1	B	329	LEU
1	B	332	LEU
1	B	349	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	ASN
1	B	280	GLN
1	B	281	ASN
1	B	305	ASN
1	B	346	HIS
1	B	349	GLN

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 carbohydrates 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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	82/104 (78%)	0.53	8 (9%) 8 11	29, 53, 102, 128	0
1	B	76/104 (73%)	0.61	5 (6%) 19 24	23, 41, 94, 114	0
All	All	158/208 (75%)	0.57	13 (8%) 12 16	23, 49, 101, 128	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	ASP	6.3
1	B	276	THR	4.5
1	B	277	GLU	4.1
1	B	274	TYR	3.9
1	B	279	LEU	3.7
1	A	348	GLN	3.4
1	B	273	ARG	3.3
1	A	267	PHE	2.8
1	A	269	GLU	2.6
1	A	340	LEU	2.6
1	A	349	GLN	2.2
1	A	339	LEU	2.0
1	A	350	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.