



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 11, 2017 – 04:17 PM EST

PDB ID : 5GJE
EMDB ID: : EMD-9501
Title : Three-dimensional reconstruction of human LRP6 ectodomain complexed with Dkk1
Authors : Matoba, K.; Mihara, E.; Tamura-Kawakami, K.; Hirai, H.; Thompson, S.; Iwasaki, K.; Takagi, J.
Deposited on : 2016-06-29
Resolution : 21.00 Å(reported)
Based on PDB ID : 3S2K, 4DG6

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

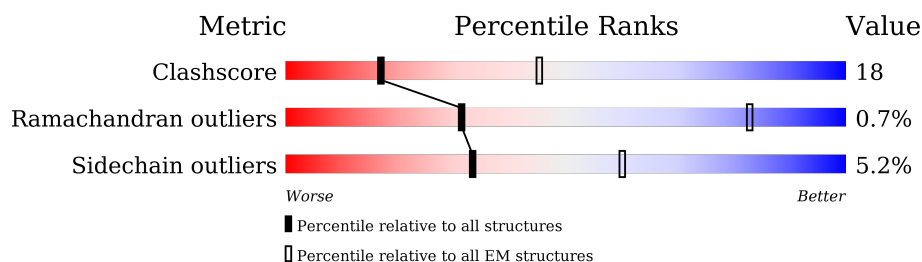
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 21.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	611	
2	B	616	
3	C	85	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10506 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	611	Total	C	N	O	S	0	0
			4856	3078	831	923	24		

- Molecule 2 is a protein called Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	606	Total	C	N	O	S	0	0
			4833	3033	856	919	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1062	ILE	VAL	engineered mutation	UNP O75581

- Molecule 3 is a protein called Dickkopf-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	76	Total	C	N	O	S	0	0
			596	362	123	101	10		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



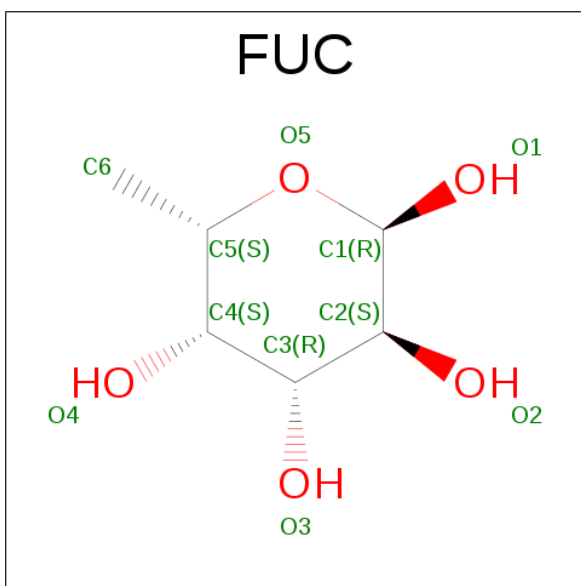
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	B	1	Total	C	N	O	0
			98	56	7	35	
4	B	1	Total	C	N	O	0
			98	56	7	35	
4	B	1	Total	C	N	O	0
			98	56	7	35	
4	B	1	Total	C	N	O	0
			98	56	7	35	
4	B	1	Total	C	N	O	0
			98	56	7	35	
4	B	1	Total	C	N	O	0
			98	56	7	35	

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	O	P	0
			10	8	2	
5	A	1	Total	O	P	0
			10	8	2	

- Molecule 6 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	C	O	0
			10	6	4	

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	C	O	0
			6	3	3	

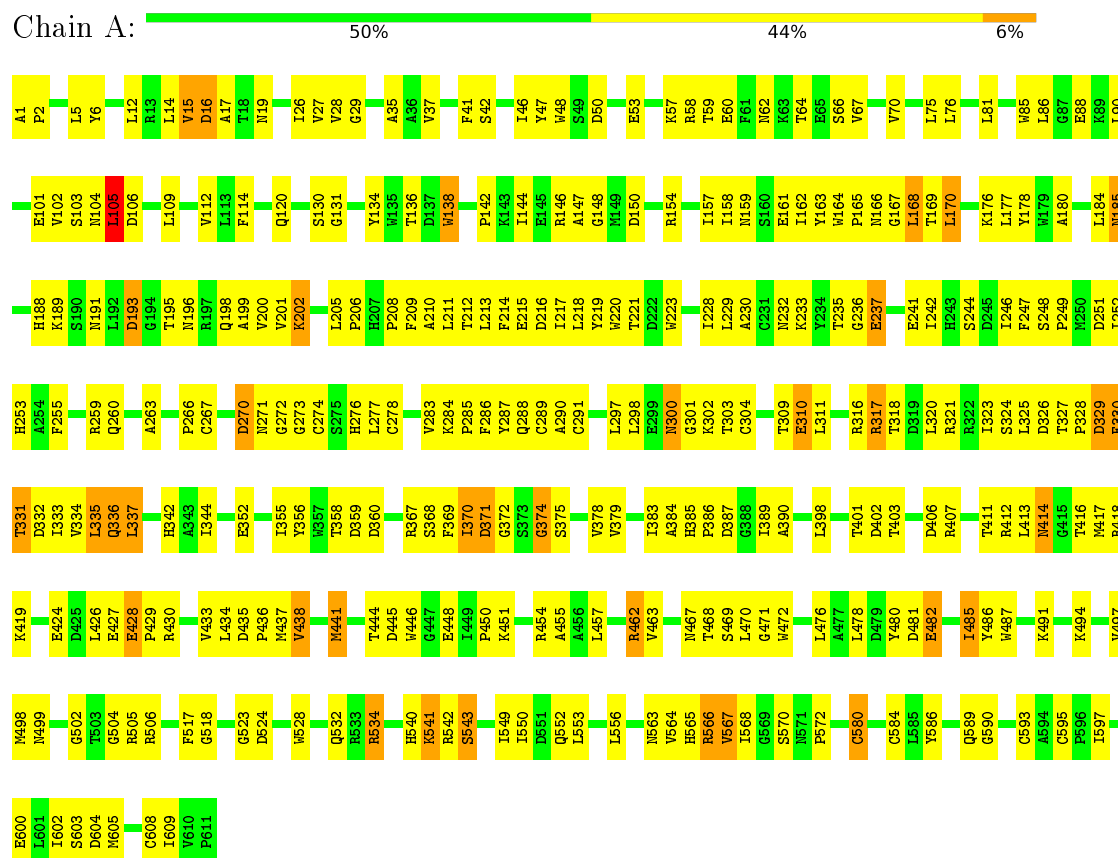
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	13	Total	O	0
			13	13	

3 Residue-property plots

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. 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: Low-density lipoprotein receptor-related protein 6



- Molecule 2: Low-density lipoprotein receptor-related protein 6





● Molecule 3: Dickkopf-related protein 1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	5390	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	HITACHI H-9500SD	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	80000	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, NAG, FUC

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 >2	RMSZ	# Z >2
1	A	0.40	0/4972	0.57	0/6766
2	B	0.23	0/4934	0.43	0/6694
3	C	0.23	0/605	0.40	0/801
All	All	0.32	0/10511	0.50	0/14261

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	VAL	Peptide
1	A	374	GLY	Peptide

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	4856	0	4726	272	0
2	B	4833	0	4711	84	0
3	C	596	0	589	16	0
4	A	84	0	75	4	0
4	B	98	0	88	2	0
5	A	10	0	0	1	0
6	B	10	0	10	0	0
7	B	6	0	8	0	0
8	A	13	0	0	0	0
All	All	10506	0	10207	369	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.

The worst 5 of 369 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:336:GLN:NE2	1:A:337:LEU:H	1.40	1.20
1:A:389:ILE:HD11	1:A:398:LEU:HD11	1.49	0.94
1:A:336:GLN:NE2	1:A:337:LEU:N	2.21	0.88
1:A:162:ILE:HB	1:A:165:PRO:HG3	1.56	0.88
2:B:773:ILE:HB	2:B:787:VAL:HG13	1.57	0.86

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 PDB entries followed by that with respect to all EM entries.

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	609/611 (100%)	505 (83%)	96 (16%)	8 (1%)	15	60
2	B	602/616 (98%)	559 (93%)	42 (7%)	1 (0%)	52	86
3	C	72/85 (85%)	67 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1283/1312 (98%)	1131 (88%)	143 (11%)	9 (1%)	31	71

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	VAL
1	A	543	SER
1	A	16	ASP
1	A	330	PHE
1	A	337	LEU

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 PDB entries followed by that with respect to all EM entries.

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	527/527 (100%)	487 (92%)	40 (8%)	16	53
2	B	529/538 (98%)	512 (97%)	17 (3%)	46	76
3	C	66/74 (89%)	65 (98%)	1 (2%)	72	88
All	All	1122/1139 (98%)	1064 (95%)	58 (5%)	33	65

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	428	GLU
1	A	485	ILE
2	B	1125	ARG
1	A	433	VAL
1	A	444	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	207	HIS

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Mol	Chain	Res	Type
1	A	336	GLN
1	A	196	ASN
1	A	300	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 ⓘ

17 ligands are modelled in this entry.

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	NAG	A	701	1,4	14,14,15	0.72	0	15,19,21	0.84	0
4	NAG	A	702	4	14,14,15	0.66	0	15,19,21	0.77	1 (6%)
4	NAG	A	703	1,4	14,14,15	0.66	0	15,19,21	0.69	0
4	NAG	A	704	4	14,14,15	0.77	0	15,19,21	0.65	0
4	NAG	A	705	1,4	14,14,15	0.80	0	15,19,21	1.19	2 (13%)
4	NAG	A	706	4	14,14,15	0.79	1 (7%)	15,19,21	0.69	0
5	PO4	A	707	-	4,4,4	1.36	0	6,6,6	0.23	0
5	PO4	A	708	-	4,4,4	1.39	0	6,6,6	0.23	0
4	NAG	B	1301	2,4,6	14,14,15	0.48	0	15,19,21	0.67	0
4	NAG	B	1302	4	14,14,15	0.46	0	15,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FUC	B	1303	4	10,10,11	0.61	0	13,14,16	0.85	1 (7%)
4	NAG	B	1304	2	14,14,15	0.46	0	15,19,21	0.83	0
4	NAG	B	1305	2	14,14,15	0.44	0	15,19,21	0.97	0
4	NAG	B	1306	2	14,14,15	0.48	0	15,19,21	0.77	0
4	NAG	B	1307	2,4	14,14,15	0.51	0	15,19,21	1.39	2 (13%)
4	NAG	B	1308	4	14,14,15	0.44	0	15,19,21	0.76	0
7	GOL	B	1309	-	5,5,5	0.38	0	5,5,5	0.18	0

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	NAG	A	701	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	702	4	-	0/6/23/26	0/1/1/1
4	NAG	A	703	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	704	4	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	706	4	-	0/6/23/26	0/1/1/1
5	PO4	A	707	-	-	0/0/0/0	0/0/0/0
5	PO4	A	708	-	-	0/0/0/0	0/0/0/0
4	NAG	B	1301	2,4,6	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	4	-	0/6/23/26	0/1/1/1
6	FUC	B	1303	4	-	0/0/17/20	0/1/1/1
4	NAG	B	1304	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	4	-	0/6/23/26	0/1/1/1
7	GOL	B	1309	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	706	NAG	C1-C2	2.31	1.55	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	NAG	C2-N2-C7	-2.46	119.90	123.11
4	A	705	NAG	C2-N2-C7	-2.39	120.00	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1303	FUC	O5-C5-C6	2.05	109.96	106.28
4	B	1307	NAG	O5-C5-C4	2.89	114.92	110.13
4	B	1307	NAG	C1-O5-C5	3.01	116.57	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	NAG	1	0
4	A	703	NAG	2	0
4	A	705	NAG	1	0
4	A	706	NAG	1	0
5	A	707	PO4	1	0
4	B	1304	NAG	1	0
4	B	1305	NAG	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.