



wwPDB X-ray Structure Validation Summary Report

Jun 10, 2014 – 10:55 AM EDT

PDB ID : 4OQT
Title : LINGO-1/Li81 Fab complex
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Deposited on : 2014-02-10
Resolution : 3.23 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

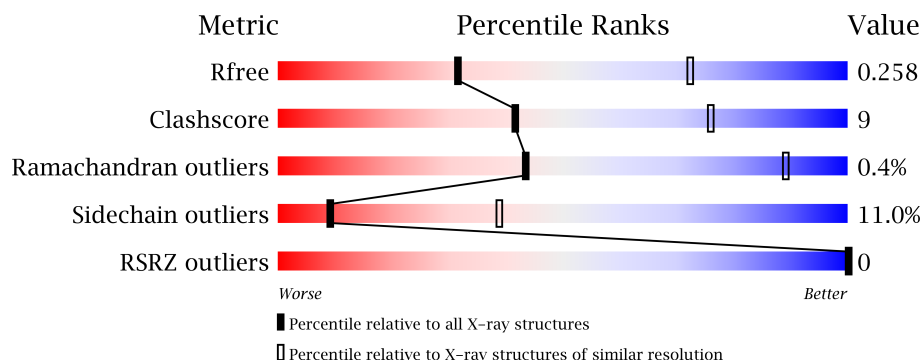
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23161
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23161

1 Overall quality at a glance

The reported resolution of this entry is 3.23 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}	66092	1080 (3.30-3.18)
Clashscore	79885	1369 (3.30-3.18)
Ramachandran outliers	78287	1342 (3.30-3.18)
Sidechain outliers	78261	1340 (3.30-3.18)
RSRZ outliers	66119	1081 (3.30-3.18)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	478	
2	L	215	
3	H	235	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	NAG	A	506	-	X
6	NAG	A	510	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7257 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Leucine-rich repeat and immunoglobulin-like domain-containing nogo receptor-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3795	2415	679	684	17			

- Molecule 2 is a protein called Light Chain of Li81 Fab, kappa 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1643	1025	278	334	6			

- Molecule 3 is a protein called Heavy Chain of Li81 Fab, VH3-23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total	C	N	O	S	0	0	0
			1618	1019	268	324	7			

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

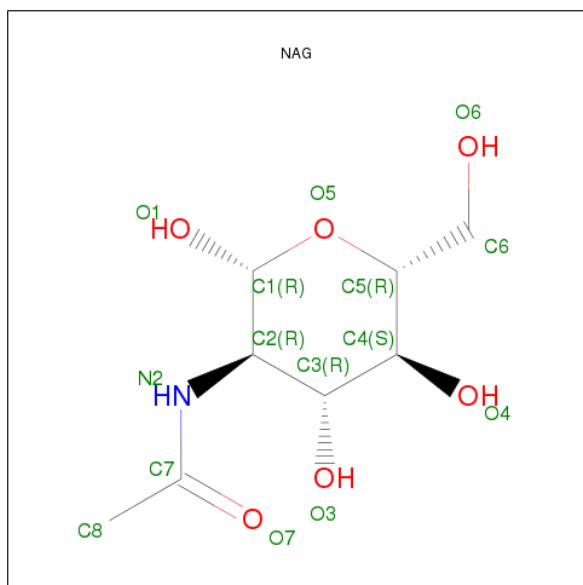
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	207.47Å 207.47Å 140.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.23 20.00 – 3.23	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.23) 100.0 (20.00-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.192 , 0.256 0.204 , 0.258	Depositor DCC
R_{free} test set	1479 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	99.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 29011 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7257	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.59	0/3877	0.88	5/5272 (0.1%)
2	L	0.60	0/1680	0.78	0/2286
3	H	0.55	0/1656	0.77	0/2259
All	All	0.58	0/7213	0.83	5/9817 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	VAL	C-N-CD	6.41	141.86	128.40
1	A	30	ILE	C-N-CD	5.77	140.52	128.40
1	A	352	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	446	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	251	ARG	NE-CZ-NH1	5.46	123.03	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3795	0	3799	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1643	0	1568	43	0
3	H	1618	0	1550	37	0
4	A	117	0	102	6	0
5	A	56	0	50	1	0
6	A	28	0	26	0	0
All	All	7257	0	7095	130	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 130 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:30:ILE:CG2	1:A:55:PHE:CE1	2.22	1.22
1:A:30:ILE:HG21	1:A:55:PHE:CE1	1.81	1.15
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.25	1.13
1:A:30:ILE:HG22	1:A:55:PHE:CE1	1.89	1.05
3:H:37:VAL:HG22	3:H:47:TRP:CE3	1.91	1.05

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	473/478 (99%)	419 (89%)	52 (11%)	2 (0%)	43	89
2	L	212/215 (99%)	196 (92%)	16 (8%)	0	100	100
3	H	219/235 (93%)	206 (94%)	11 (5%)	2 (1%)	25	77
All	All	904/928 (97%)	821 (91%)	79 (9%)	4 (0%)	43	89

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ALA

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Mol	Chain	Res	Type
3	H	178	SER
3	H	103	ASP
1	A	470	PRO

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	423/428 (99%)	375 (89%)	48 (11%)	9	37
2	L	183/187 (98%)	162 (88%)	21 (12%)	8	37
3	H	177/196 (90%)	160 (90%)	17 (10%)	12	46
All	All	783/811 (96%)	697 (89%)	86 (11%)	9	39

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	404	GLN
2	L	3	GLN
3	H	135	SER
1	A	421	SER
1	A	436	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
2	L	167	GLN
2	L	6	GLN
1	A	349	ASN
2	L	139	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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, 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	475/478 (99%)	-0.34	0 100 100	66, 88, 132, 164	0
2	L	214/215 (99%)	-0.26	0 100 100	68, 93, 123, 138	0
3	H	221/235 (94%)	-0.20	0 100 100	59, 103, 130, 152	0
All	All	910/928 (98%)	-0.29	0 100 100	59, 93, 128, 164	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	A	502	14/15	0.35	5.43	74,98,107,127	0
5	NAG	A	505	14/15	0.33	4.26	114,131,145,155	0
5	NAG	A	512	14/15	0.28	2.97	97,129,142,157	0
4	NAG	A	514	14/15	0.29	2.95	70,81,90,101	0
4	NAG	A	508	14/15	0.20	0.68	76,84,100,127	0
5	NAG	A	511	14/15	0.15	-0.13	90,98,105,106	0
5	NAG	A	504	14/15	0.17	-0.30	75,84,90,95	0
4	NAG	A	501	14/15	0.15	-0.52	73,77,85,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	513	14/15	0.12	-0.87	65,73,78,78	0
4	NAG	A	507	14/15	0.12	-1.91	78,89,98,106	0
4	BMA	A	509	11/12	0.23	-	100,112,125,131	0
4	BMA	A	503	11/12	0.29	-	98,121,155,176	0
4	BMA	A	515	11/12	0.31	-	95,114,126,135	0

6.4 Ligands

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	A	506	14/15	0.50	7.02	114,138,156,159	0
6	NAG	A	510	14/15	0.33	2.92	113,142,163,171	0

6.5 Other polymers

There are no such residues in this entry.