



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5A5C
Title : Structure of an engineered neuronal LRRTM2 adhesion molecule
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Deposited on : 2015-06-17
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure 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/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

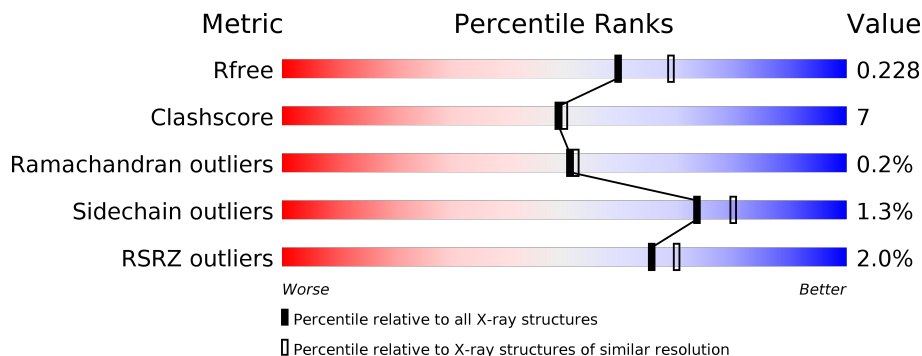
1 Overall quality at a glance

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	357	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 11%, yellow 11%, green 80%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 6% 80% 11% 8% </div> </div>
1	B	357	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 13%, yellow 13%, green 80%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 1% 80% 13% 7% </div> </div>
1	C	357	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 9%, yellow 9%, green 82%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 1% 82% 9% 8% </div> </div>
1	D	357	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 11%, yellow 11%, green 80%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 6% 80% 11% 8% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20811 atoms, of which 10133 are hydrogens and 0 are deuteriums.

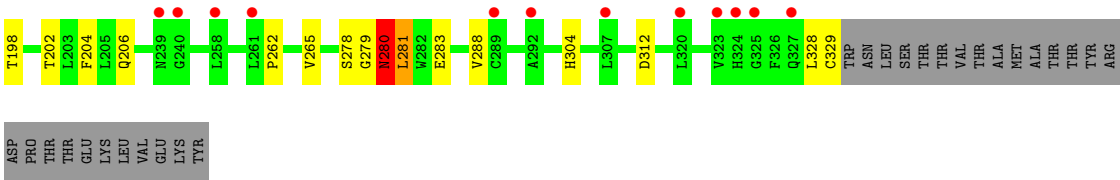
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LRRTM.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	H	N	O	S	0	0	0
			5140	1638	2563	444	487	8			
1	B	332	Total	C	H	N	O	S	0	0	0
			5159	1650	2566	442	492	9			
1	C	329	Total	C	H	N	O	S	0	0	0
			5062	1619	2514	437	484	8			
1	D	329	Total	C	H	N	O	S	0	0	0
			5029	1614	2490	432	484	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	133	Total	O	0	0
			133	133		
2	B	139	Total	O	0	0
			139	139		
2	C	104	Total	O	0	0
			104	104		
2	D	45	Total	O	0	0
			45	45		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.99Å 57.32Å 144.45Å 90.00° 115.49° 90.00°	Depositor
Resolution (Å)	44.74 – 2.10 44.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.74-2.10) 99.6 (44.74-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.195 , 0.236 0.186 , 0.228	Depositor DCC
R_{free} test set	5074 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20811	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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

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	0.73	0/2631	0.85	8/3583 (0.2%)
1	B	0.72	0/2650	0.80	6/3612 (0.2%)
1	C	0.68	1/2601 (0.0%)	0.77	3/3546 (0.1%)
1	D	0.63	0/2593	0.78	6/3538 (0.2%)
All	All	0.69	1/10475 (0.0%)	0.80	23/14279 (0.2%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	308	CYS	CB-SG	-5.79	1.72	1.81

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	PHE	C-N-CA	7.66	140.86	121.70
1	A	27	GLY	N-CA-C	-7.40	94.61	113.10
1	D	280	ASN	C-N-CA	7.30	139.96	121.70
1	D	280	ASN	CA-C-N	6.87	132.31	117.20
1	A	41	GLN	N-CA-C	-6.83	92.57	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	280	ASN	Peptide

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	2577	2563	2552	44	0
1	B	2593	2566	2555	38	0
1	C	2548	2514	2502	27	0
1	D	2539	2490	2479	36	0
2	A	133	0	0	6	0
2	B	139	0	0	7	0
2	C	104	0	0	3	0
2	D	45	0	0	1	0
All	All	10678	10133	10088	138	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 7.

The worst 5 of 138 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:41:GLN:O	1:A:42:LEU:HB2	1.48	1.07
1:A:298:PHE:HA	1:A:299:GLN:HG2	1.49	0.93
1:A:298:PHE:CD1	1:A:299:GLN:HG2	2.10	0.87
1:D:279:GLY:HA2	1:D:280:ASN:HB2	1.56	0.86
1:A:298:PHE:CD1	1:A:299:GLN:CG	2.58	0.85

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	328/357 (92%)	304 (93%)	22 (7%)	2 (1%)	28	24
1	B	330/357 (92%)	311 (94%)	19 (6%)	0	100	100
1	C	327/357 (92%)	305 (93%)	22 (7%)	0	100	100
1	D	327/357 (92%)	306 (94%)	20 (6%)	1 (0%)	44	44
All	All	1312/1428 (92%)	1226 (93%)	83 (6%)	3 (0%)	51	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	D	281	LEU
1	A	299	GLN

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	299/330 (91%)	295 (99%)	4 (1%)	73	80
1	B	301/330 (91%)	296 (98%)	5 (2%)	66	72
1	C	293/330 (89%)	291 (99%)	2 (1%)	87	91
1	D	292/330 (88%)	288 (99%)	4 (1%)	71	78
All	All	1185/1320 (90%)	1170 (99%)	15 (1%)	73	80

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	LEU
1	B	86	SER
1	D	42	LEU
1	B	33	LEU
1	D	28	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	183	HIS
1	C	39	HIS
1	C	309	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.

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	330/357 (92%)	0.00	2 (0%) 89 91	29, 50, 73, 95	0
1	B	332/357 (92%)	-0.06	2 (0%) 89 91	30, 47, 71, 82	0
1	C	329/357 (92%)	-0.16	3 (0%) 84 86	33, 51, 76, 94	0
1	D	329/357 (92%)	0.32	20 (6%) 22 27	40, 63, 87, 108	0
All	All	1320/1428 (92%)	0.03	27 (2%) 65 70	29, 52, 80, 108	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.3
1	D	325	GLY	4.0
1	B	-1	GLY	3.9
1	D	323	VAL	3.7
1	D	324	HIS	3.4

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.