



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 06:28 PM JST

PDB ID : 6LI5
Title : Crystal structure of apo-MCR-1-S
Authors : Zhang, Q.; Wang, M.; Sun, H.
Deposited on : 2019-12-10
Resolution : 1.82 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

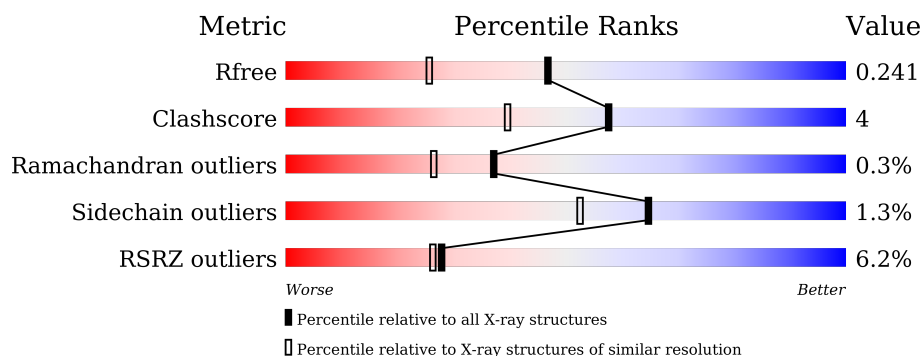
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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}	164625	9242 (1.84-1.80)
Clashscore	180529	1080 (1.82-1.82)
Ramachandran outliers	177936	1073 (1.82-1.82)
Sidechain outliers	177891	1073 (1.82-1.82)
RSRZ outliers	164620	9241 (1.84-1.80)

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 $\leq 5\%$. 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	323	
1	B	323	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5196 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 Probable phosphatidylethanolamine transferase Mcr-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	P	S	2	7	0
			2564	1614	428	505	1	16			
1	B	323	Total	C	N	O	P	S	0	5	0
			2558	1609	428	504	1	16			

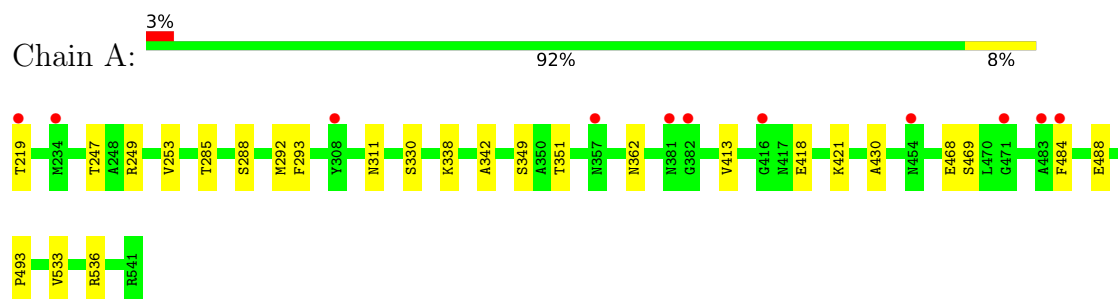
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total	O	0	0
			55	55		
2	B	19	Total	O	0	0
			19	19		

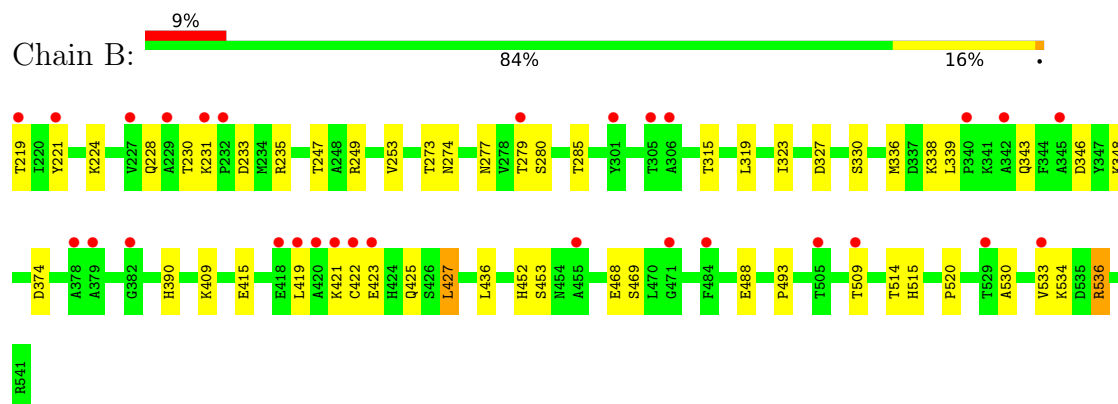
3 Residue-property plots [i](#)

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 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: Probable phosphatidylethanolamine transferase Mcr-1



- Molecule 1: Probable phosphatidylethanolamine transferase Mcr-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.16Å 84.05Å 81.42Å 90.00° 98.51° 90.00°	Depositor
Resolution (Å)	40.78 – 1.82 40.78 – 1.82	Depositor EDS
% Data completeness (in resolution range)	90.6 (40.78-1.82) 90.7 (40.78-1.82)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.200 , 0.243 0.201 , 0.241	Depositor DCC
R_{free} test set	2737 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5196	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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

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

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	0.42	0/2630	0.58	0/3569
1	B	0.35	0/2618	0.52	0/3551
All	All	0.39	0/5248	0.55	0/7120

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	A	2564	0	2465	16	0
1	B	2558	0	2456	33	0
2	A	55	0	0	0	0
2	B	19	0	0	1	0
All	All	5196	0	4921	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 4.

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:A:351:THR:HG22	1:B:509:THR:HG21	1.56	0.87
1:A:351:THR:HG22	1:B:509:THR:CG2	2.04	0.86
1:B:415:GLU:H	1:B:421:LYS:HE3	1.65	0.61
1:B:274:ASN:O	1:B:509:THR:HB	2.02	0.60
1:A:413:VAL:HG13	1:A:430:ALA:HB2	1.84	0.59
1:B:249:ARG:HD2	1:B:468:GLU:O	2.03	0.58
1:B:315:THR:O	1:B:319:LEU:HD12	2.03	0.58
1:A:351:THR:CG2	1:B:509:THR:HG21	2.32	0.57
1:B:423:GLU:OE2	1:B:425:GLN:HB3	2.07	0.54
1:A:533:VAL:HA	1:A:536:ARG:HG3	1.90	0.54
1:B:228:GLN:OE1	1:B:231:LYS:HE2	2.08	0.54
1:A:249:ARG:HD2	1:A:468:GLU:O	2.09	0.53
1:A:418:GLU:HG2	1:A:421:LYS:HB2	1.91	0.51
1:B:279:THR:OG1	1:B:514:THR:HG22	2.11	0.51
1:B:221:TYR:CD1	1:B:224:LYS:HG2	2.46	0.51
1:B:273:THR:HG23	1:B:509:THR:HG22	1.92	0.51
1:B:469:SER:HA	1:B:488[A]:GLU:HG3	1.92	0.51
1:A:247:THR:HG22	1:A:247:THR:O	2.12	0.50
1:B:520:PRO:HG3	1:B:536:ARG:HG2	1.93	0.50
1:B:533:VAL:C	1:B:534:LYS:HE2	2.32	0.49
1:B:346:ASP:OD1	1:B:348:LYS:NZ	2.40	0.49
1:A:469:SER:HA	1:A:488[A]:GLU:HG3	1.95	0.49
1:B:419:LEU:HD23	1:B:427:LEU:HD13	1.95	0.48
1:B:231:LYS:HB2	1:B:233:ASP:OD1	2.15	0.47
1:B:253:VAL:HG21	1:B:493:PRO:HB3	1.97	0.47
1:B:374:ASP:OD1	1:B:452:HIS:NE2	2.43	0.46
1:A:288:SER:O	1:A:292:MET:HG3	2.16	0.45
1:B:323:ILE:O	1:B:343:GLN:HB3	2.16	0.45
1:A:219:THR:HG21	1:A:338:LYS:HD3	1.99	0.45
1:B:219:THR:HG21	1:B:338:LYS:HD3	1.98	0.45
1:A:351:THR:O	1:B:509:THR:HG23	2.17	0.45
1:B:336:MET:SD	1:B:339:LEU:HD12	2.57	0.45
1:B:536:ARG:NH2	2:B:603:HOH:O	2.49	0.45
1:A:253:VAL:HG21	1:A:493:PRO:HB3	1.98	0.45
1:B:409[B]:LYS:HD3	1:B:436:LEU:HD13	1.98	0.45
1:B:530:ALA:O	1:B:534:LYS:HE3	2.17	0.45
1:B:247:THR:O	1:B:247:THR:HG22	2.16	0.44
1:A:293:PHE:O	1:A:311:ASN:HB2	2.17	0.44
1:B:230:THR:HB	1:B:235:ARG:HG2	1.99	0.43
1:A:342:ALA:HB1	1:B:277:ASN:HB2	2.01	0.42
1:B:280:SER:HB2	1:B:515:HIS:CE1	2.55	0.41
1:B:273:THR:CG2	1:B:509:THR:HG22	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ASP:OD2	1:B:390:HIS:ND1	2.44	0.41
1:A:418:GLU:HG2	1:A:418:GLU:O	2.22	0.40

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	327/323 (101%)	315 (96%)	11 (3%)	1 (0%)	37	26
1	B	325/323 (101%)	314 (97%)	10 (3%)	1 (0%)	37	26
All	All	652/646 (101%)	629 (96%)	21 (3%)	2 (0%)	37	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	330	SER
1	A	330	SER

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	280/274 (102%)	277 (99%)	3 (1%)	70	59
1	B	279/274 (102%)	275 (99%)	4 (1%)	62	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	559/548 (102%)	552 (99%)	7 (1%)	65	52

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	SER
1	A	362	ASN
1	A	484	PHE
1	B	422	CYS
1	B	427	LEU
1	B	453	SER
1	B	536	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	A	362	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	285	1	8,10,11	1.89	2 (25%)	10,14,16	1.74	1 (10%)
1	TPO	B	285	1	8,10,11	1.80	1 (12%)	10,14,16	1.68	1 (10%)

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
1	TPO	A	285	1	-	1/9/11/13	-
1	TPO	B	285	1	-	1/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	TPO	P-O1P	3.83	1.62	1.50
1	A	285	TPO	P-O1P	3.54	1.62	1.50
1	A	285	TPO	P-OG1	2.85	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	TPO	P-OG1-CB	-4.81	108.66	123.21
1	B	285	TPO	P-OG1-CB	-4.80	108.72	123.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	285	TPO	O-C-CA-CB
1	B	285	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

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	322/323 (99%)	0.28	11 (3%) 48 48	25, 41, 60, 71	8 (2%)
1	B	322/323 (99%)	1.01	29 (9%) 17 15	33, 55, 79, 104	5 (1%)
All	All	644/646 (99%)	0.65	40 (6%) 28 26	25, 48, 74, 104	13 (2%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	419	LEU	6.2
1	B	420	ALA	4.5
1	A	484	PHE	4.4
1	B	533	VAL	3.7
1	A	308	TYR	3.5
1	B	227	VAL	3.4
1	B	509	THR	3.1
1	B	422	CYS	3.0
1	B	279	THR	3.0
1	B	471	GLY	2.9
1	B	418	GLU	2.8
1	A	483	ALA	2.7
1	B	219	THR	2.6
1	B	340	PRO	2.6
1	A	219	THR	2.6
1	B	529	THR	2.6
1	B	382	GLY	2.6
1	B	345	ALA	2.6
1	B	423	GLU	2.5
1	B	484	PHE	2.5
1	B	306	ALA	2.4
1	B	379	ALA	2.4
1	A	234	MET	2.4
1	B	421	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	357	ASN	2.3
1	B	232	PRO	2.3
1	B	301	TYR	2.3
1	B	378	ALA	2.3
1	B	342	ALA	2.3
1	A	471	GLY	2.3
1	B	231	LYS	2.2
1	B	305	THR	2.2
1	A	382	GLY	2.2
1	A	416	GLY	2.1
1	B	505	THR	2.1
1	B	229	ALA	2.1
1	A	381	ASN	2.1
1	B	221	TYR	2.1
1	B	455	ALA	2.0
1	A	454	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	B	285	11/12	0.85	0.14	53,56,77,78	0
1	TPO	A	285	11/12	0.90	0.12	35,47,60,65	1

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.