

wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 12:53 am GMT

PDB ID	:	8AYF
Title	:	Crystal structure of human Sphingosine-1-phosphate lyase 1
Authors	:	Giardina, G.; Catalano, F.; Pampalone, G.; Cellini, B.
Deposited on		
Resolution	:	1.84 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

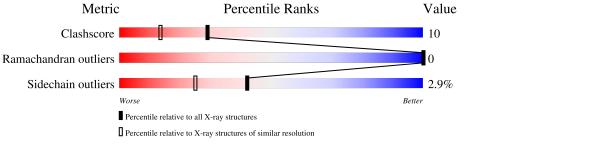
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain			
1	А	494	76%	13%	·	10%
1	В	494	77%	13%	·	9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	А	601[A]	-	-	Х	-
2	ACT	А	601[B]	-	-	Х	-
2	ACT	В	601[A]	-	-	Х	-

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		Chain	1 0	Chirality	Geometry	Clashes	Electron density
2	ACT	В	601[B]	-	-	Х	-
3	GOL	В	602	-	-	Х	-

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2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7239 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.

Mol	Chain	Residues		I	Atom	s			ZeroOcc	AltConf	Trace
1	А	443	Total 3449	C 2216					3	3	0
1	В	448	Total 3443	C 2208		O 638	Р 1	S 22	0	1	0

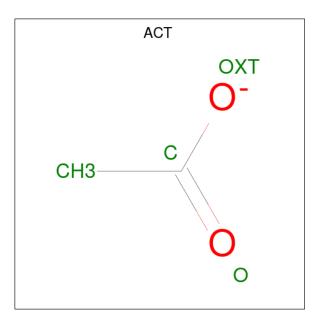
• Molecule 1 is a protein called Sphingosine-1-phosphate lyase 1.

Chain	Residue	Modelled	Actual	Comment	Reference
А	569	HIS	-	expression tag	UNP O95470
А	570	HIS	-	expression tag	UNP 095470
А	571	HIS	-	expression tag	UNP O95470
А	572	HIS	-	expression tag	UNP O95470
А	573	HIS	-	expression tag	UNP O95470
А	574	HIS	-	expression tag	UNP O95470
В	569	HIS	-	expression tag	UNP O95470
В	570	HIS	-	expression tag	UNP O95470
В	571	HIS	-	expression tag	UNP O95470
В	572	HIS	-	expression tag	UNP O95470
В	573	HIS	-	expression tag	UNP O95470
В	574	HIS	-	expression tag	UNP O95470

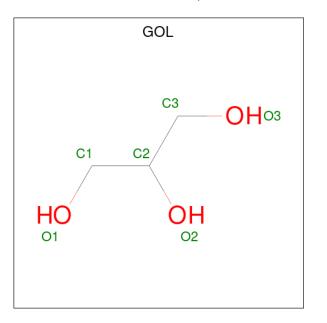
There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 4 & 4 \end{array}$	0	1
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 4 & 4 \end{array}$	0	1



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	148	Total O 148 148	0	0
4	В	171	Total O 171 171	0	0



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. 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.

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1.00/

Note EDS failed to run properly.

• Molecule 1: Sphingosine-1-phosphate lyase 1 Chain A:

											/0																	10%				
MET PRO ILE	ILE GLY ARG LYS TIFE	GLN	LYS	LYS	THR LYS	ASP	ILE	SER	ASN	NET	PHE	LYS	VAL ASP	LYS	1	L116	K131 F130	Y133	M136		6147	T148 V149	Y150	R182	K183	1188	A192	V FC F	1771	K228	T232 P233	E234
1235 V236 A237	S240 A241 N246	M254	K255 1256	V257 R258	L261	T080	A281	CORF		4289 F290	P291 1707	6293	V294 1295	D296	C317	1323	F337		D350 T351	H352	CCCN	P358	L363	<mark>0375</mark>	7387		A403	K421	1424	G439	T451	
D457	N473 L474 N475 D476	L477 Q478	H484	F485	T488 L489	L490 H401	1491	1498	N514	0530		D534	M537 V538		L541 S542	S543	8551 TEEO	1002 D553	THR VAL	THR	GLY	SER GLN	MET	ALC N	PRO	LYS	PRO HIS	HIS	SIH	SIH	HIS	
• M	olecule	1	a									_																				
• 1010	Jiecule	9 1:	Sp	hi	ngo	osi	ne	<u>-1</u>	-p]	ho	sp	ha	ite	ly	ase	e 1	-															
	n B: •	91:	Sp	hi	ngo	osi	ne	÷-1	-p]	hos		ha 7%	ıte	ly	as	e 1	-						-	13	%		·	9%)			
Chai											77	7%		ly		R144	A145	G180	L181 B182		Q217	L195	L215	13 13	P233 %		•	H242 M243	A244	A248	K255	-
Chai	n B: •		LYS							MET SER	77	7%		1361 5361 5361	K370 F139	Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q	A145	4.000 G180	S389 L181 R182	R396	A403	L195 E413			1424 P233 %	K431	5432 A237 • E433	H242 MAAN	477 A244	N445 P446 A248	Q447 K355	F458



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	59.16Å 127.41Å 66.95Å	Depositor
a, b, c, α , β , γ	90.00° 104.85° 90.00°	Depositor
Resolution (Å)	57.76 - 1.84	Depositor
% Data completeness	57.3 (57.76-1.84)	Depositor
(in resolution range)	· · · · · · · · · · · · · · · · · · ·	-
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.55 (at 1.84 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.191 , 0.214	Depositor
Wilson B-factor $(Å^2)$	18.8	Xtriage
Anisotropy	0.032	Xtriage
L-test for twinning ²	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7239	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.30% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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, ACT, LLP

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 Chair		Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.43	0/3506	0.71	1/4749~(0.0%)	
1	В	0.44	0/3499	0.69	0/4746	
All	All	0.44	0/7005	0.70	1/9495~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	182	ARG	NE-CZ-NH1	-5.31	117.64	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	А	3449	0	3402	60	0
1	В	3443	0	3373	70	0
2	А	8	0	6	6	0
2	В	8	0	6	5	0
3	А	6	0	8	0	0
3	В	6	0	8	6	0
4	А	148	0	0	23	0
4	В	171	0	0	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7239	0	6803	132	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 10.

The worst 5 of 132 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)
2:A:601[B]:ACT:H1	4:A:839:HOH:O	1.43	1.18
2:A:601[B]:ACT:H2	4:A:841:HOH:O	1.51	1.08
1:A:317:CYS:SG	4:A:704:HOH:O	2.19	1.01
1:A:131:LYS:CG	4:A:817:HOH:O	2.13	0.94
1:B:442:VAL:HB	4:B:822:HOH:O	1.66	0.93

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	А	443/494~(90%)	433 (98%)	10 (2%)	0	100 100
1	В	446/494~(90%)	433 (97%)	13 (3%)	0	100 100
All	All	889/988~(90%)	866 (97%)	23 (3%)	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 side chain 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.



Mol	Chain	Analysed	ysed Rotameric		Percentiles
1	А	360/414~(87%)	351 (98%)	9~(2%)	47 31
1	В	357/414 (86%)	345~(97%)	12 (3%)	37 19
All	All	717/828~(87%)	696~(97%)	21 (3%)	42 25

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

5 of 21 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	352	HIS
1	В	473	ASN
1	В	490	LEU
1	В	476	GLN
1	В	375	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	473	ASN
1	В	478	GLN
1	В	491	HIS
1	В	476	GLN
1	А	499	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)

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).



Mal	Mol Type Chain Res L		Link	Bo	ond leng	$_{\rm ths}$	В	ond ang	les	
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	LLP	В	353	1	$23,\!24,\!25$	0.82	1 (4%)	$25,\!32,\!34$	1.10	1 (4%)
1	LLP	А	353	1	23,24,25	0.76	1 (4%)	25,32,34	1.13	2 (8%)

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	LLP	В	353	1	-	11/16/17/19	0/1/1/1
1	LLP	А	353	1	-	10/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	353	LLP	C4'-NZ	2.31	1.35	1.27
1	В	353	LLP	C4'-NZ	2.01	1.34	1.27

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$\operatorname{Ideal}(^{o})$
1	А	353	LLP	OP3-P-OP4	-2.15	101.00	106.73
1	В	353	LLP	C5-C4-C4'	2.09	124.99	121.56
1	А	353	LLP	OP3-P-OP2	2.05	115.46	107.64

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	353	LLP	C4-C4'-NZ-CE
1	А	353	LLP	C4-C5-C5'-OP4
1	А	353	LLP	C6-C5-C5'-OP4
1	А	353	LLP	C5'-OP4-P-OP2
1	А	353	LLP	C5'-OP4-P-OP3

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	353	LLP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	353	LLP	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	Mal Trung Chain Dag Lir		Res Link G Bond lengths					Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	В	602	-	$5,\!5,\!5$	0.21	0	$5,\!5,\!5$	0.66	0
2	ACT	А	601[A]	-	3,3,3	0.90	0	$3,\!3,\!3$	0.78	0
2	ACT	В	601[A]	-	3,3,3	0.92	0	$3,\!3,\!3$	0.95	0
2	ACT	А	601[B]	-	3,3,3	0.68	0	$3,\!3,\!3$	1.15	0
2	ACT	В	601[B]	-	3,3,3	0.72	0	$3,\!3,\!3$	0.95	0
3	GOL	А	602	-	$5,\!5,\!5$	0.15	0	$5,\!5,\!5$	0.32	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
3	GOL	А	602	-	-	0/4/4/4	-
3	GOL	В	602	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	В	602	GOL	O1-C1-C2-C3
3	В	602	GOL	C1-C2-C3-O3
3	В	602	GOL	O2-C2-C3-O3
3	В	602	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	602	GOL	6	0
2	А	601[A]	ACT	3	0
2	В	601[A]	ACT	2	0
2	А	601[B]	ACT	3	0
2	В	601[B]	ACT	3	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.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

