



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2017 – 11:14 AM EST

PDB ID : 5M0J
Title : Crystal structure of the cytoplasmic complex with She2p, She3p, and the ASH1 mRNA E3-localization element
Authors : Edelman, F.T.; Janowski, R.; Niessing, D.
Deposited on : 2016-10-05
Resolution : 2.80 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

<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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	rb-20028442

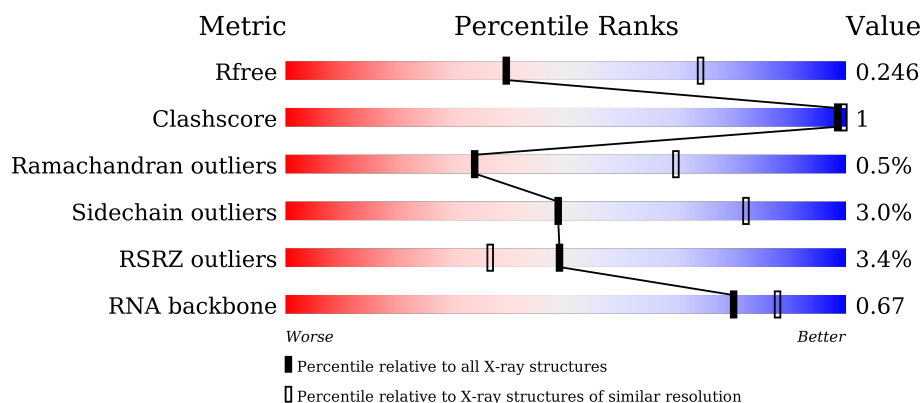
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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	328	<div> <div>2%</div> <div>64%</div> <div>32%</div> </div>
1	B	328	<div> <div>2%</div> <div>69%</div> <div>29%</div> </div>
1	C	328	<div> <div>0%</div> <div>70%</div> <div>27%</div> </div>
1	D	328	<div> <div>2%</div> <div>65%</div> <div>5%</div> <div>29%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	328	
1	H	328	
1	I	328	
1	J	328	
2	E	28	
2	F	28	

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
3	MG	A	401	-	-	-	X
3	MG	B	401	-	-	-	X
3	MG	C	401	-	-	-	X
3	MG	D	401	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9621 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 SWI5-dependent HO expression protein 2,SWI5-dependent HO expression protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	232	Total	C	N	O	S	0	3	0
			1914	1231	307	374	2			
1	C	240	Total	C	N	O	S	0	1	0
			1952	1257	313	380	2			
1	B	234	Total	C	N	O	S	0	2	0
			1920	1238	310	370	2			
1	A	223	Total	C	N	O	S	0	0	0
			1811	1172	289	348	2			
1	J	21	Total	C	N	O		0	0	0
			170	109	34	27				
1	G	16	Total	C	N	O		0	0	0
			127	80	25	22				
1	H	22	Total	C	N	O		0	0	0
			171	108	34	29				
1	I	20	Total	C	N	O		0	0	0
			153	101	27	25				

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	4	GLY	-	expression tag	UNP B3LQW9
D	5	PRO	-	expression tag	UNP B3LQW9
D	14	SER	CYS	engineered mutation	UNP B3LQW9
D	68	SER	CYS	engineered mutation	UNP B3LQW9
D	106	SER	CYS	engineered mutation	UNP B3LQW9
D	180	SER	CYS	engineered mutation	UNP B3LQW9
D	247	GLY	-	linker	UNP B3LQW9
D	248	GLY	-	linker	UNP B3LQW9
D	249	SER	-	linker	UNP B3LQW9
D	250	GLY	-	linker	UNP B3LQW9
D	251	GLY	-	linker	UNP B3LQW9
D	252	GLY	-	linker	UNP B3LQW9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	253	GLY	-	linker	UNP B3LQW9
D	254	SER	-	linker	UNP B3LQW9
D	255	GLY	-	linker	UNP B3LQW9
D	256	GLY	-	linker	UNP B3LQW9
C	4	GLY	-	expression tag	UNP B3LQW9
C	5	PRO	-	expression tag	UNP B3LQW9
C	14	SER	CYS	engineered mutation	UNP B3LQW9
C	68	SER	CYS	engineered mutation	UNP B3LQW9
C	106	SER	CYS	engineered mutation	UNP B3LQW9
C	180	SER	CYS	engineered mutation	UNP B3LQW9
C	247	GLY	-	linker	UNP B3LQW9
C	248	GLY	-	linker	UNP B3LQW9
C	249	SER	-	linker	UNP B3LQW9
C	250	GLY	-	linker	UNP B3LQW9
C	251	GLY	-	linker	UNP B3LQW9
C	252	GLY	-	linker	UNP B3LQW9
C	253	GLY	-	linker	UNP B3LQW9
C	254	SER	-	linker	UNP B3LQW9
C	255	GLY	-	linker	UNP B3LQW9
C	256	GLY	-	linker	UNP B3LQW9
B	4	GLY	-	expression tag	UNP B3LQW9
B	5	PRO	-	expression tag	UNP B3LQW9
B	14	SER	CYS	engineered mutation	UNP B3LQW9
B	68	SER	CYS	engineered mutation	UNP B3LQW9
B	106	SER	CYS	engineered mutation	UNP B3LQW9
B	180	SER	CYS	engineered mutation	UNP B3LQW9
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B	248	GLY	-	linker	UNP B3LQW9
B	249	SER	-	linker	UNP B3LQW9
B	250	GLY	-	linker	UNP B3LQW9
B	251	GLY	-	linker	UNP B3LQW9
B	252	GLY	-	linker	UNP B3LQW9
B	253	GLY	-	linker	UNP B3LQW9
B	254	SER	-	linker	UNP B3LQW9
B	255	GLY	-	linker	UNP B3LQW9
B	256	GLY	-	linker	UNP B3LQW9
A	4	GLY	-	expression tag	UNP B3LQW9
A	5	PRO	-	expression tag	UNP B3LQW9
A	14	SER	CYS	engineered mutation	UNP B3LQW9
A	68	SER	CYS	engineered mutation	UNP B3LQW9
A	106	SER	CYS	engineered mutation	UNP B3LQW9
A	180	SER	CYS	engineered mutation	UNP B3LQW9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	247	GLY	-	linker	UNP B3LQW9
A	248	GLY	-	linker	UNP B3LQW9
A	249	SER	-	linker	UNP B3LQW9
A	250	GLY	-	linker	UNP B3LQW9
A	251	GLY	-	linker	UNP B3LQW9
A	252	GLY	-	linker	UNP B3LQW9
A	253	GLY	-	linker	UNP B3LQW9
A	254	SER	-	linker	UNP B3LQW9
A	255	GLY	-	linker	UNP B3LQW9
A	256	GLY	-	linker	UNP B3LQW9
J	78	GLY	-	expression tag	UNP B3LQW9
J	79	PRO	-	expression tag	UNP B3LQW9
J	88	SER	CYS	engineered mutation	UNP B3LQW9
J	142	SER	CYS	engineered mutation	UNP B3LQW9
J	180	SER	CYS	engineered mutation	UNP B3LQW9
J	254	SER	CYS	engineered mutation	UNP B3LQW9
J	321	GLY	-	linker	UNP B3LQW9
J	322	GLY	-	linker	UNP B3LQW9
J	323	SER	-	linker	UNP B3LQW9
J	324	GLY	-	linker	UNP B3LQW9
J	325	GLY	-	linker	UNP B3LQW9
J	326	GLY	-	linker	UNP B3LQW9
J	327	GLY	-	linker	UNP B3LQW9
J	328	SER	-	linker	UNP B3LQW9
J	329	GLY	-	linker	UNP B3LQW9
J	330	GLY	-	linker	UNP B3LQW9
G	78	GLY	-	expression tag	UNP B3LQW9
G	79	PRO	-	expression tag	UNP B3LQW9
G	88	SER	CYS	engineered mutation	UNP B3LQW9
G	142	SER	CYS	engineered mutation	UNP B3LQW9
G	180	SER	CYS	engineered mutation	UNP B3LQW9
G	254	SER	CYS	engineered mutation	UNP B3LQW9
G	321	GLY	-	linker	UNP B3LQW9
G	322	GLY	-	linker	UNP B3LQW9
G	323	SER	-	linker	UNP B3LQW9
G	324	GLY	-	linker	UNP B3LQW9
G	325	GLY	-	linker	UNP B3LQW9
G	326	GLY	-	linker	UNP B3LQW9
G	327	GLY	-	linker	UNP B3LQW9
G	328	SER	-	linker	UNP B3LQW9
G	329	GLY	-	linker	UNP B3LQW9
G	330	GLY	-	linker	UNP B3LQW9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	78	GLY	-	expression tag	UNP B3LQW9
H	79	PRO	-	expression tag	UNP B3LQW9
H	88	SER	CYS	engineered mutation	UNP B3LQW9
H	142	SER	CYS	engineered mutation	UNP B3LQW9
H	180	SER	CYS	engineered mutation	UNP B3LQW9
H	254	SER	CYS	engineered mutation	UNP B3LQW9
H	321	GLY	-	linker	UNP B3LQW9
H	322	GLY	-	linker	UNP B3LQW9
H	323	SER	-	linker	UNP B3LQW9
H	324	GLY	-	linker	UNP B3LQW9
H	325	GLY	-	linker	UNP B3LQW9
H	326	GLY	-	linker	UNP B3LQW9
H	327	GLY	-	linker	UNP B3LQW9
H	328	SER	-	linker	UNP B3LQW9
H	329	GLY	-	linker	UNP B3LQW9
H	330	GLY	-	linker	UNP B3LQW9
I	78	GLY	-	expression tag	UNP B3LQW9
I	79	PRO	-	expression tag	UNP B3LQW9
I	88	SER	CYS	engineered mutation	UNP B3LQW9
I	142	SER	CYS	engineered mutation	UNP B3LQW9
I	180	SER	CYS	engineered mutation	UNP B3LQW9
I	254	SER	CYS	engineered mutation	UNP B3LQW9
I	321	GLY	-	linker	UNP B3LQW9
I	322	GLY	-	linker	UNP B3LQW9
I	323	SER	-	linker	UNP B3LQW9
I	324	GLY	-	linker	UNP B3LQW9
I	325	GLY	-	linker	UNP B3LQW9
I	326	GLY	-	linker	UNP B3LQW9
I	327	GLY	-	linker	UNP B3LQW9
I	328	SER	-	linker	UNP B3LQW9
I	329	GLY	-	linker	UNP B3LQW9
I	330	GLY	-	linker	UNP B3LQW9

- Molecule 2 is a RNA chain called ASH1 E3 (28 nt-loop).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	28	Total	C	N	O	P	0	0	0
			596	269	112	188	27			
2	F	28	Total	C	N	O	P	0	0	0
			596	269	112	188	27			

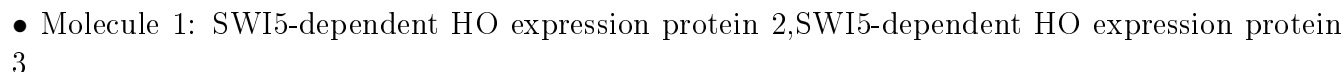
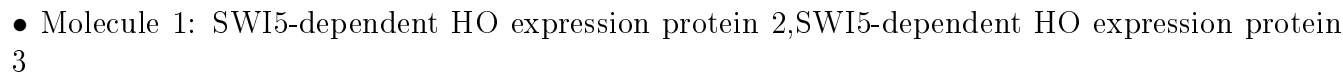
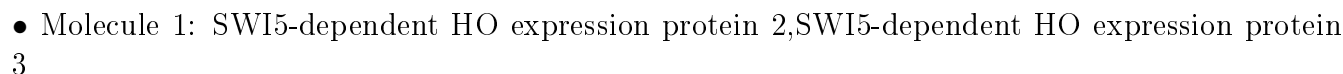
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

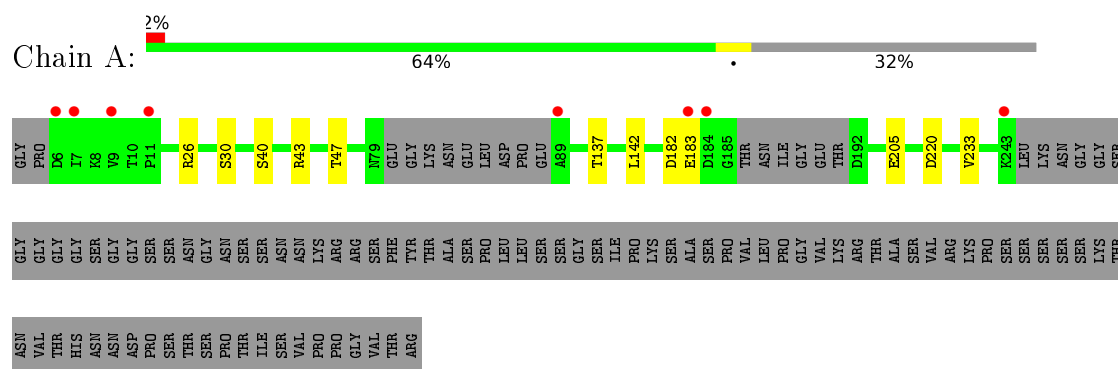
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is water.

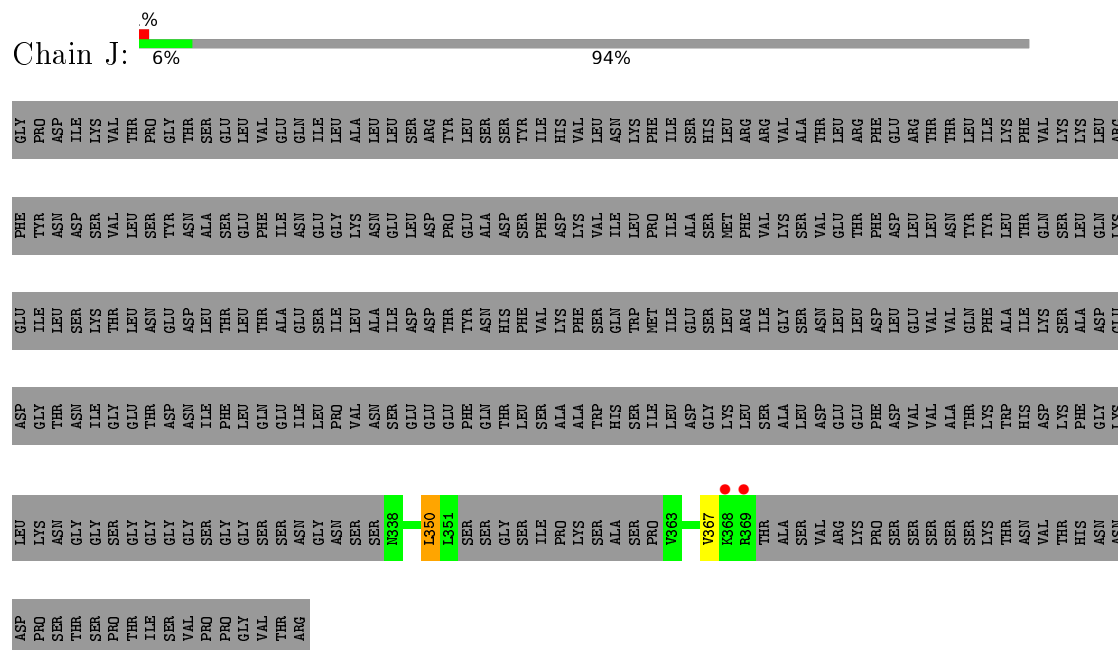
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	39	Total O 39 39	0	0
4	C	37	Total O 37 37	0	0
4	B	45	Total O 45 45	0	0
4	A	33	Total O 33 33	0	0
4	J	3	Total O 3 3	0	0
4	G	1	Total O 1 1	0	0
4	H	5	Total O 5 5	0	0
4	I	5	Total O 5 5	0	0
4	E	19	Total O 19 19	0	0
4	F	20	Total O 20 20	0	0

● Molecule 1: SWI5-dependent HO expression protein 2,SWI5-dependent HO expression protein

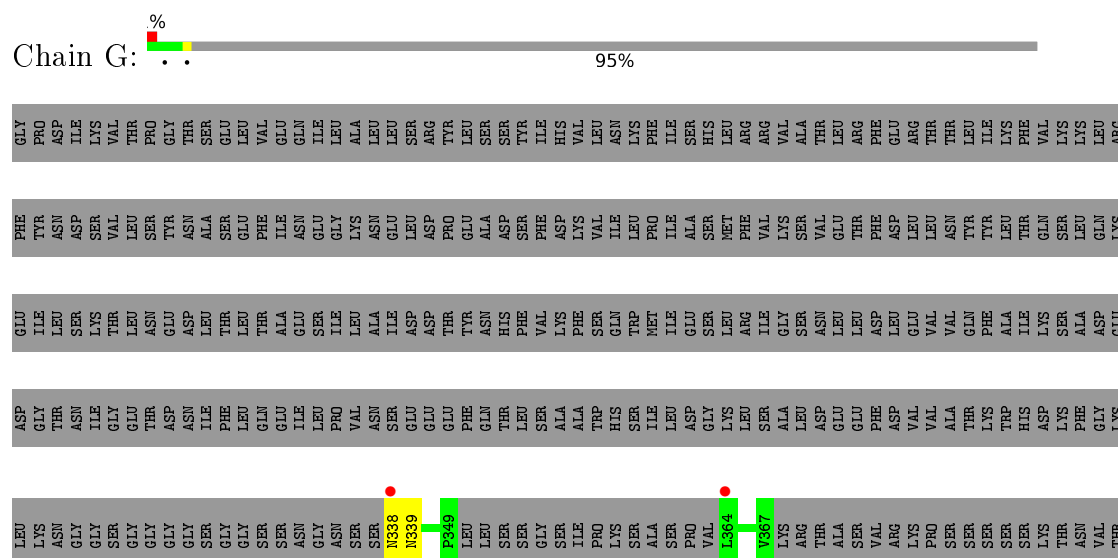




- Molecule 1: SWI5-dependent HO expression protein 2,SWI5-dependent HO expression protein



- Molecule 1: SWI5-dependent HO expression protein 2,SWI5-dependent HO expression protein



HIS
ASN
ASN
ASP
PRO
SER
THR
SER
PRO
THR
ILE
SER
VAL
PRO
PRO
GLY
VAL
THR
ARG

- Molecule 1: SWI5-dependent HO expression protein 2,SWI5-dependent HO expression protein

[illegible]

PHE	TYR	ASN	ASP	SER	VAL	LEU	LEU	SER	TYR	ASN	ALA	SER	GLU	PHE	ILE	ASN	GLY	LYS	ASN	GLU	LEU	ASP	PRO	GLU	GLU	ALA	ASP	PHE	ASP	LYS	VAL	ILE	LEU	PRO	ILE	ALA	SER	SER	MET	PHE	VAL	LYS	PHE	THR	GLN	LEU	TYR	ASN	LEU	LEU	GLN	GLN
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GLU ILE LEU LEU SER LYS THR LEU LEU ASN GLU ASP LEU THR LEU THR GLU ALA SER ILE LEU ALA ASP THR THR TRP MET ILE GLU LEU SER LEU ARG ILE GLY SER ASN LEU LEU ASP LEU VAL VAL VAL GLN PHE ALA ILE LYS ILE SER ASP

ASP	GLY	THR	ASN	ILE	GLY	GLU	THR	ASP	ASN	ASP	PHE	LEU	GLN	GLU	ILE	LEU	PRO	VAL	ASN	SER	GLU	GLU	GLU	GLU	PHE	GLN	THR	LEU	SER	ALA	ALA	TRP	THR	ASP	GLY	LYS	LEU	SER	ALA	ASP	GLU	GLU	PHE	ASP	VAL	VAL	ALA	ALA	THR	LYS	THR	ASP	PHE	GLY
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LEU LYS ASN LYS GLY GLY SER GLY GLY GLY SER GLY GLY SER SER SER SER ASN GLY ASN SER SER SER SER SER SER SER S361 P362 V363 K368 R369 A371 SER VAL ARG LYS PRO SER SER SER SER SER LYS THR ASN VAL THR HIS

ASN
ASP
PRO
SER
THR
SER
PRO
THR
ILE
SER
VAL
PRO
PRO
GLY
VAL
THR
ARG

- Molecule 1: SWI5-dependent HO expression protein 2,SWI5-dependent HO expression protein



GLY	PRO	ASP	ILE	LYS	VAL	THR	PRO	GLY	THR	SER	GLU	LEU	GLU	VAL	GLU	GLN	ILE	LEU	ALA	LEU	LEU	SER	SER	TYR	ILE	ILE	HIS	VAL	LEU	ASN	LYS	PHE	ILE	SER	HIS	LEU	ARG	ARG	VAL	ALA	THR	THR	THR	THR	LEU	ILE	LYS	PHE	VAL	LYS	LYS	LEU
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PHE TYR ASN ASP SER VAL LEU SER TYR ASN ALA SER PHE ILE PHE ASN GLY LYS ASN LEU ASP PRAO GLU ALA ASP ASP PHE PHE LYS VAL ILE LEU PRO ILE ALA SER SER MET PHE PHE VAL LYS SER VAL GLU PHE LEU ASN TYR TYR LEU THR SER GLN

GLU
ILE
LEU
SER
LYS
THR
LEU
ASN
GLU
ASP
LEU
THR
LEU
THR
THR
ALA
GLU
SER
ILE
LEU
ALA
ILE
ASP
ASP
THR
TYR
ASN
HIS
PHE
VAL
LYS
PHE
SER
GLN
TRP
MET
ILE
GLU
LEU
SER
ARG
ILE
GLY
SER
ASN
LEU
LEU
ASP
LEU
VAL
VAL
GLN
PHE
ALA
ILE
LYS
SER
ALA
ASP

ASP	GLY	THR	ASN	ILE	ILE	GLY	GLU	GLU	THR	ASP	ASN	ASN	ILE	PHE	LEU	GLU	GLN	GLU	ILE	LEU	PRO	VAL	ASN	SER	GLU	GLU	PHE	THR	GLN	THR	LEU	SER	ALA	ALA	TRP	TRP	SER	HIS	ASP	ASP	GLY	LYS	LEU	SER	ALA	LEU	ASP	ASP	GLU	GLU	PHE	ASP	VAL	VAL	ALA	THR	THR	LYS	TRP	HIS	ASP	PHE	LYS	GLY
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LEU	LVS	ASN	GLY	GLY	SER	GLY	GLY	GLY	GLY	SER	GLY	SER	SER	ASN	ASN	ASN	ASN	LVS	ARG	R342	R350	R351	SER	SER	GLY	GLY	ILE	PRO	LVS	SER	ALA	ALA	SER	P362	V363	V364	A371	VAL	ARG	LVS	PRO	SER	SER	SER	SER	LVS	THR	ASN	VAL	THR	HIS
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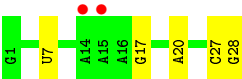
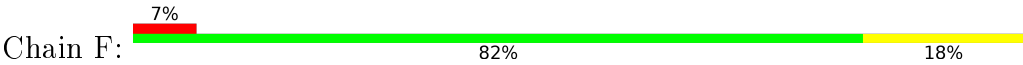
ASN
ASP
PRO
SER
THR
SER
PRO
THR
ILE
SER
VAL
PRO
PRO
GLY
VAL
THR
ARG

- Molecule 2: ASH1 E3 (28 nt-loop)





● Molecule 2: ASH1 E3 (28 nt-loop)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.03Å 58.98Å 144.68Å 90.00° 126.91° 90.00°	Depositor
Resolution (Å)	50.01 – 2.80 47.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.01-2.80) 100.0 (47.29-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.194 , 0.246 0.198 , 0.246	Depositor DCC
R_{free} test set	1828 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.8	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	0.94	EDS
Total number of atoms	9621	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: MG

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	0.53	0/1844	0.74	2/2494 (0.1%)
1	B	0.58	0/1956	0.76	0/2645
1	C	0.57	0/1989	0.72	0/2693
1	D	0.58	0/1950	0.78	1/2640 (0.0%)
1	G	0.68	0/129	0.88	0/172
1	H	0.72	0/174	0.90	0/233
1	I	0.67	0/156	0.83	0/210
1	J	0.69	0/172	0.99	0/229
2	E	0.56	0/668	0.91	4/1039 (0.4%)
2	F	0.51	0/668	0.81	0/1039
All	All	0.57	0/9706	0.78	7/13394 (0.1%)

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	B	0	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ARG	NE-CZ-NH1	-7.93	116.33	120.30
1	A	26	ARG	NE-CZ-NH2	7.13	123.86	120.30
2	E	7	U	N1-C1'-C2'	6.87	122.93	114.00
2	E	26	A	N9-C1'-C2'	6.38	122.29	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	26	A	O4'-C1'-N9	6.22	113.18	108.20
2	E	17	G	O5'-P-OP2	5.66	117.49	110.70
1	D	197	GLN	CB-CA-C	5.08	120.57	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	ASP	Peptide
1	D	82	LYS	Peptide
1	D	85	LEU	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	1811	0	1811	4	0
1	B	1920	0	1916	2	0
1	C	1952	0	1945	3	0
1	D	1914	0	1892	8	0
1	G	127	0	126	0	0
1	H	171	0	179	0	0
1	I	153	0	165	1	0
1	J	170	0	183	2	0
2	E	596	0	304	1	0
2	F	596	0	304	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	33	0	0	0	0
4	B	45	0	0	1	0
4	C	37	0	0	0	0
4	D	39	0	0	1	0
4	E	19	0	0	0	0
4	F	20	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	J	3	0	0	0	0
All	All	9621	0	8825	16	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 1.

All (16) 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:D:197:GLN:HG3	1:J:367:VAL:HG13	1.78	0.65
1:C:191:THR:HG21	1:C:196:LEU:HB2	1.83	0.60
1:D:191:THR:HG21	1:D:196:LEU:HB2	1.85	0.58
1:D:47:THR:HG21	1:A:47:THR:HG21	1.89	0.53
1:D:197:GLN:HG3	1:J:367:VAL:CG1	2.44	0.47
1:A:40:SER:O	1:A:43:ARG:HB2	2.17	0.45
1:C:10:THR:HG23	1:C:205:GLU:OE1	2.18	0.44
1:B:83:ASN:N	1:B:83:ASN:OD1	2.52	0.43
1:B:43[B]:ARG:NH1	4:B:503:HOH:O	2.51	0.42
1:D:10:THR:HG23	1:D:205:GLU:OE1	2.19	0.42
2:E:9:A:C2	2:E:10:A:C4	3.06	0.42
1:D:47:THR:CG2	1:A:47:THR:HG21	2.50	0.41
1:D:49[A]:ARG:NH1	4:D:502:HOH:O	2.53	0.41
1:C:215:TRP:CH2	1:I:364:LEU:HD22	2.56	0.41
1:D:86:ASP:N	1:D:86:ASP:OD1	2.50	0.41
1:A:137:THR:HG23	1:A:233:VAL:HG12	2.02	0.41

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	217/328 (66%)	213 (98%)	4 (2%)	0	100	100
1	B	232/328 (71%)	226 (97%)	5 (2%)	1 (0%)	39	74
1	C	239/328 (73%)	235 (98%)	3 (1%)	1 (0%)	39	74
1	D	231/328 (70%)	223 (96%)	6 (3%)	2 (1%)	21	55
1	G	12/328 (4%)	12 (100%)	0	0	100	100
1	H	18/328 (6%)	16 (89%)	2 (11%)	0	100	100
1	I	16/328 (5%)	16 (100%)	0	0	100	100
1	J	17/328 (5%)	14 (82%)	2 (12%)	1 (6%)	2	5
All	All	982/2624 (37%)	955 (97%)	22 (2%)	5 (0%)	34	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	83	ASN
1	C	84	GLU
1	J	350	LEU
1	B	84	GLU
1	D	7	ILE

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	205/292 (70%)	199 (97%)	6 (3%)	50	83
1	B	217/292 (74%)	212 (98%)	5 (2%)	58	88
1	C	221/292 (76%)	217 (98%)	4 (2%)	66	91
1	D	217/292 (74%)	210 (97%)	7 (3%)	46	80
1	G	14/292 (5%)	12 (86%)	2 (14%)	4	12
1	H	19/292 (6%)	17 (90%)	2 (10%)	8	24
1	I	17/292 (6%)	16 (94%)	1 (6%)	24	57
1	J	19/292 (6%)	18 (95%)	1 (5%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	929/2336 (40%)	901 (97%)	28 (3%)	48 82

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	30	SER
1	D	44	ARG
1	D	80	GLU
1	D	84	GLU
1	D	142	LEU
1	D	182	ASP
1	D	190	GLU
1	C	30	SER
1	C	80	GLU
1	C	142	LEU
1	C	182	ASP
1	B	30	SER
1	B	80	GLU
1	B	84	GLU
1	B	142	LEU
1	B	182	ASP
1	A	30	SER
1	A	142	LEU
1	A	182	ASP
1	A	183	GLU
1	A	205	GLU
1	A	220	ASP
1	J	350	LEU
1	G	338	ASN
1	G	339	ASN
1	H	363	VAL
1	H	368	LYS
1	I	350	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	C	66	ASN
1	B	66	ASN
1	A	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	27/28 (96%)	4 (14%)	0
2	F	27/28 (96%)	5 (18%)	0
All	All	54/56 (96%)	9 (16%)	0

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	7	U
2	E	20	A
2	E	27	C
2	E	28	G
2	F	7	U
2	F	17	G
2	F	20	A
2	F	27	C
2	F	28	G

There are no RNA pucker outliers to report.

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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	223/328 (67%)	-0.07	8 (3%)	46	34	23, 50, 98, 118	1 (0%)
1	B	234/328 (71%)	-0.28	6 (2%)	59	47	20, 40, 94, 121	1 (0%)
1	C	240/328 (73%)	-0.22	4 (1%)	73	63	23, 39, 90, 134	0
1	D	232/328 (70%)	-0.22	8 (3%)	49	36	20, 41, 95, 141	0
1	G	16/328 (4%)	0.37	2 (12%)	5	2	33, 80, 98, 106	0
1	H	22/328 (6%)	0.37	3 (13%)	4	2	45, 68, 109, 126	0
1	I	20/328 (6%)	0.61	1 (5%)	32	21	35, 66, 94, 103	0
1	J	21/328 (6%)	0.33	2 (9%)	10	5	33, 62, 108, 114	0
2	E	28/28 (100%)	0.02	0	100	100	31, 45, 69, 77	0
2	F	28/28 (100%)	0.12	2 (7%)	19	10	28, 42, 78, 82	0
All	All	1064/2680 (39%)	-0.14	36 (3%)	49	36	20, 43, 98, 141	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	ASN	5.6
1	A	11	PRO	4.9
1	C	83	ASN	4.8
1	C	81	GLY	4.0
1	I	350	LEU	3.5
1	A	89	ALA	3.5
1	D	87	PRO	3.4
1	A	184	ASP	3.3
1	B	87	PRO	3.3
1	H	371	ALA	3.2
1	H	370	THR	3.1
1	B	83	ASN	3.0
1	C	87	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	84	GLU	2.9
1	D	191	THR	2.8
1	J	369	ARG	2.8
1	B	6	ASP	2.8
1	D	181	ALA	2.8
1	A	6	ASP	2.7
1	D	6	ASP	2.6
2	F	14	A	2.5
1	J	368	LYS	2.5
1	A	7	ILE	2.5
1	A	243	LYS	2.5
1	G	338	ASN	2.4
1	A	9	VAL	2.4
1	D	184	ASP	2.4
1	B	185	GLY	2.3
1	H	339	ASN	2.2
1	D	192	ASP	2.1
1	G	364	LEU	2.1
1	B	85	LEU	2.1
1	A	183	GLU	2.1
1	B	182	ASP	2.1
2	F	15	A	2.0
1	D	11	PRO	2.0

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](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	A	401	1/1	0.95	0.52	24.04	70,70,70,70	0
3	MG	C	401	1/1	0.98	0.46	23.30	54,54,54,54	0
3	MG	D	401	1/1	0.95	0.52	19.25	62,62,62,62	0
3	MG	B	401	1/1	0.98	0.45	13.80	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.