



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:35 am GMT

PDB ID : 2E31
Title : Structural basis for selection of glycosylated substrate by SCFFbs1 ubiquitin ligase
Authors : Mizushima, T.; Yoshida, Y.; Kumanomidou, T.; Hasegawa, Y.; Yamane, T.; Tanaka, K.
Deposited on : 2006-11-20
Resolution : 2.40 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
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

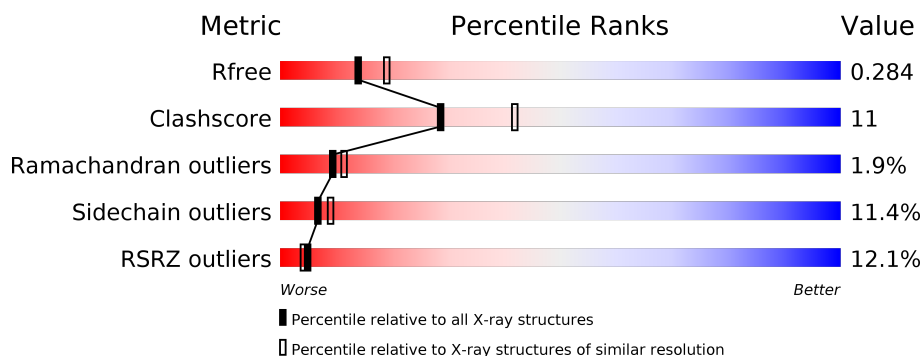
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	297	<div> <div>3%</div> <div>66%</div> <div>14%</div> <div>••</div> <div>17%</div> </div>
2	B	166	<div> <div>22%</div> <div>49%</div> <div>23%</div> <div>7%</div> <div>•</div> <div>20%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3077 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 F-box only protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1997	1277	333	381	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	LYS	ARG	SEE REMARK 999	UNP Q80UW2

- Molecule 2 is a protein called S-phase kinase-associated protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1058	674	171	209	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	CLONING ARTIFACT	UNP P63208
B	-1	PRO	-	CLONING ARTIFACT	UNP P63208
B	0	HIS	-	CLONING ARTIFACT	UNP P63208

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.41Å 106.41Å 109.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.22 – 2.40 53.20 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (53.22-2.40) 97.8 (53.20-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.233 , 0.291 0.230 , 0.284	Depositor DCC
R_{free} test set	1425 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3077	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.51	0/2052	0.67	0/2791
2	B	0.47	0/1073	0.64	1/1449 (0.1%)
All	All	0.50	0/3125	0.66	1/4240 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	34	LEU	CA-CB-CG	7.46	132.47	115.30

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	A	1997	0	1890	39	0
2	B	1058	0	1068	32	0
3	A	21	0	0	0	0
3	B	1	0	0	0	0
All	All	3077	0	2958	66	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 11.

All (66) 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:129:ARG:HH11	1:A:129:ARG:HG2	1.31	0.96
1:A:54:LEU:HD11	2:B:104:ILE:HD11	1.52	0.92
1:A:207:VAL:HG11	1:A:225:VAL:HG21	1.57	0.85
1:A:129:ARG:HH11	1:A:129:ARG:CG	1.91	0.83
2:B:51:ASN:C	2:B:51:ASN:HD22	1.84	0.81
1:A:112:ASP:O	1:A:113:HIS:HB2	1.85	0.77
1:A:247:GLU:HG2	1:A:248:ASP:H	1.52	0.75
1:A:157:GLY:HA3	1:A:287:ARG:HH12	1.52	0.75
1:A:54:LEU:HD11	2:B:104:ILE:CD1	2.17	0.73
1:A:129:ARG:NH1	1:A:129:ARG:HG2	2.02	0.72
2:B:43:ASP:N	2:B:44:PRO:HD3	2.05	0.72
1:A:54:LEU:CD1	2:B:104:ILE:HD11	2.23	0.68
2:B:127:ILE:HG23	2:B:135:ILE:HG21	1.76	0.67
2:B:51:ASN:ND2	2:B:54:ILE:H	1.95	0.65
1:A:133:GLY:O	1:A:135:GLU:O	2.15	0.64
2:B:136:ARG:HA	2:B:141:ILE:HG23	1.80	0.64
2:B:7:GLN:HG3	2:B:13:ILE:HD13	1.83	0.59
2:B:134:GLU:O	2:B:138:THR:HG23	2.02	0.59
2:B:56:LYS:O	2:B:59:ILE:HD13	2.02	0.59
1:A:247:GLU:HG2	1:A:248:ASP:N	2.16	0.58
2:B:115:LEU:O	2:B:119:THR:HG22	2.04	0.57
1:A:207:VAL:HG21	1:A:225:VAL:HG11	1.86	0.57
1:A:228:LEU:HB2	1:A:267:PHE:HB2	1.86	0.57
2:B:17:ASP:HB2	2:B:20:ILE:HD13	1.87	0.56
1:A:77:LEU:HD22	2:B:149:GLU:HB3	1.86	0.56
2:B:51:ASN:ND2	2:B:51:ASN:C	2.58	0.55
1:A:116:GLN:NE2	1:A:201:THR:HG21	2.21	0.55
1:A:240:THR:HG21	1:A:254:ILE:HD13	1.89	0.54
1:A:240:THR:CG2	1:A:254:ILE:HD13	2.37	0.54
2:B:51:ASN:HD21	2:B:54:ILE:H	1.55	0.53
2:B:153:VAL:C	2:B:155:LYS:H	2.11	0.53
2:B:55:LEU:O	2:B:59:ILE:HG23	2.09	0.52
2:B:84:ASP:O	2:B:85:ILE:HG12	2.09	0.52
1:A:51:LEU:O	1:A:52:ALA:HB2	2.10	0.51
1:A:207:VAL:HG22	1:A:293:VAL:HG22	1.92	0.51
2:B:43:ASP:N	2:B:44:PRO:CD	2.75	0.50
1:A:157:GLY:HA3	1:A:287:ARG:NH1	2.23	0.49
2:B:49:ASN:HB2	2:B:109:TYR:CE2	2.47	0.49
1:A:93:LEU:O	1:A:93:LEU:HD22	2.13	0.48
1:A:113:HIS:CE1	1:A:115:GLN:HB3	2.49	0.48
1:A:113:HIS:HB3	1:A:116:GLN:HB3	1.96	0.48
2:B:154:ARG:O	2:B:155:LYS:CB	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:VAL:O	2:B:154:ARG:HG2	2.15	0.45
2:B:131:THR:O	2:B:135:ILE:HG12	2.17	0.45
1:A:78:VAL:HG22	2:B:135:ILE:HG13	1.99	0.45
1:A:185:VAL:HG22	1:A:269:ARG:HG3	1.98	0.44
1:A:125:ARG:NH2	1:A:191:GLU:OE1	2.50	0.44
1:A:240:THR:CG2	1:A:254:ILE:CD1	2.96	0.44
2:B:26:THR:HG23	2:B:111:ASP:HB2	2.00	0.43
2:B:101:PHE:O	2:B:104:ILE:HD13	2.19	0.43
2:B:91:GLU:HA	2:B:94:LYS:HG3	2.00	0.43
1:A:240:THR:HG22	1:A:254:ILE:CD1	2.49	0.43
1:A:129:ARG:NH1	1:A:129:ARG:CG	2.63	0.42
1:A:165:GLN:HE21	1:A:165:GLN:HA	1.83	0.42
1:A:51:LEU:O	1:A:52:ALA:CB	2.67	0.42
2:B:101:PHE:CE2	2:B:105:LEU:HD11	2.55	0.41
1:A:211:TYR:HA	1:A:287:ARG:O	2.20	0.41
1:A:165:GLN:HE21	1:A:165:GLN:CA	2.33	0.41
2:B:54:ILE:O	2:B:58:VAL:HG23	2.20	0.41
1:A:238:PHE:CE2	1:A:254:ILE:HD11	2.56	0.41
1:A:119:PHE:O	1:A:123:ARG:HB2	2.21	0.41
2:B:6:LEU:HD12	2:B:45:VAL:HG12	2.01	0.41
1:A:213:GLY:N	1:A:245:VAL:HG11	2.35	0.41
2:B:117:ASP:O	2:B:121:LYS:HB2	2.21	0.40
1:A:89:ALA:N	1:A:90:PRO:CD	2.84	0.40
1:A:116:GLN:OE1	1:A:201:THR:OG1	2.40	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	242/297 (82%)	228 (94%)	10 (4%)	4 (2%)	11 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	127/166 (76%)	109 (86%)	15 (12%)	3 (2%)	7	7
All	All	369/463 (80%)	337 (91%)	25 (7%)	7 (2%)	9	11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	247	GLU
2	B	154	ARG
1	A	52	ALA
1	A	112	ASP
2	B	34	LEU
2	B	85	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	211/250 (84%)	194 (92%)	17 (8%)	14	21
2	B	121/152 (80%)	100 (83%)	21 (17%)	2	2
All	All	332/402 (83%)	294 (89%)	38 (11%)	7	9

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	65	GLU
1	A	69	THR
1	A	83	LYS
1	A	91	LEU
1	A	93	LEU
1	A	109	GLU
1	A	112	ASP
1	A	129	ARG

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Mol	Chain	Res	Type
1	A	164	THR
1	A	165	GLN
1	A	231	ASN
1	A	243	VAL
1	A	247	GLU
1	A	254	ILE
1	A	260	ASP
1	A	272	HIS
2	B	4	ILE
2	B	13	ILE
2	B	20	ILE
2	B	28	LYS
2	B	30	MET
2	B	34	LEU
2	B	50	VAL
2	B	51	ASN
2	B	59	ILE
2	B	66	LYS
2	B	68	ASP
2	B	83	ASP
2	B	104	ILE
2	B	115	LEU
2	B	121	LYS
2	B	135	ILE
2	B	138	THR
2	B	141	ILE
2	B	144	ASP
2	B	147	GLU
2	B	150	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	98	GLN
1	A	115	GLN
1	A	130	ASN
1	A	165	GLN
1	A	242	GLN
2	B	49	ASN
2	B	51	ASN
2	B	60	GLN

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Mol	Chain	Res	Type
2	B	152	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](#)

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	246/297 (82%)	0.35	10 (4%) 38 36	37, 51, 79, 94	0
2	B	133/166 (80%)	1.31	36 (27%) 1 1	63, 88, 126, 135	0
All	All	379/463 (81%)	0.69	46 (12%) 5 4	37, 59, 114, 135	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	34	LEU	10.2
2	B	59	ILE	6.9
1	A	47	ALA	6.3
2	B	31	LEU	5.5
2	B	20	ILE	5.5
2	B	63	THR	5.2
2	B	85	ILE	5.0
2	B	3	SER	4.4
1	A	157	GLY	4.2
1	A	103	PRO	3.9
2	B	35	GLY	3.8
2	B	4	ILE	3.6
2	B	92	PHE	3.5
2	B	58	VAL	3.5
2	B	2	PRO	3.5
2	B	67	ASP	3.3
2	B	44	PRO	3.2
2	B	87	VAL	3.2
1	A	48	VAL	3.1
2	B	88	TRP	3.0
2	B	16	VAL	3.0
2	B	95	VAL	2.9
1	A	50	TYR	2.9
2	B	13	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	101	PHE	2.9
2	B	32	GLU	2.8
2	B	18	VAL	2.8
1	A	162	GLU	2.8
1	A	160	GLY	2.7
2	B	33	ASP	2.7
2	B	19	GLU	2.6
2	B	15	GLU	2.6
1	A	161	VAL	2.6
2	B	21	ALA	2.6
2	B	66	LYS	2.5
2	B	91	GLU	2.5
1	A	51	LEU	2.4
2	B	45	VAL	2.3
2	B	104	ILE	2.3
2	B	84	ASP	2.2
2	B	112	ILE	2.2
1	A	167	ASP	2.1
2	B	140	ASN	2.1
2	B	23	GLN	2.1
2	B	27	ILE	2.1
2	B	118	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.