



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2025 – 12:11 PM JST

PDB ID : 8XO8
Title : Crystal structure of measles virus fusion inhibitor MEK35GT complexed with F protein HR1 (HR1-42) (P21 space group)
Authors : Oishi, S.; Takahara, A.; Nakatsu, T.
Deposited on : 2023-12-31
Resolution : 1.85 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

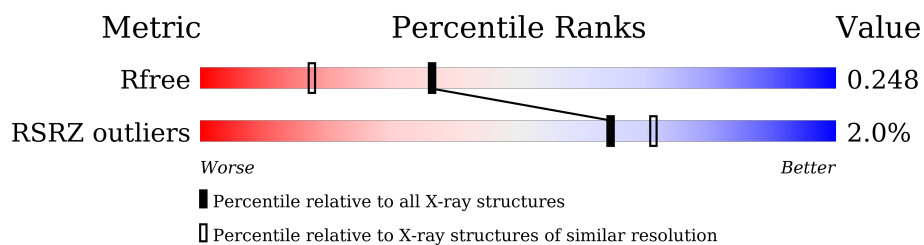
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1150 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4366 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 Fusion glycoprotein F1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	44	Total	C	N	O	S	0	5	1
			353	214	64	73	2			
1	C	44	Total	C	N	O	S	0	3	1
			341	206	62	71	2			
1	E	44	Total	C	N	O	S	0	5	1
			356	215	65	74	2			
1	G	44	Total	C	N	O	S	0	4	1
			347	210	64	71	2			
1	I	44	Total	C	N	O	S	0	4	1
			346	211	62	71	2			
1	K	44	Total	C	N	O	S	0	5	1
			352	213	62	75	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ACE	-	acetylation	UNP P69353
A	185	NH2	-	amidation	UNP P69353
C	142	ACE	-	acetylation	UNP P69353
C	185	NH2	-	amidation	UNP P69353
E	142	ACE	-	acetylation	UNP P69353
E	185	NH2	-	amidation	UNP P69353
G	142	ACE	-	acetylation	UNP P69353
G	185	NH2	-	amidation	UNP P69353
I	142	ACE	-	acetylation	UNP P69353
I	185	NH2	-	amidation	UNP P69353
K	142	ACE	-	acetylation	UNP P69353
K	185	NH2	-	amidation	UNP P69353

- Molecule 2 is a protein called Measles virus fusion inhibitor MEK35GT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	34	Total	C	N	O	0	7	1
			316	202	51	63			
2	D	37	Total	C	N	O	0	4	1
			333	211	58	64			
2	F	34	Total	C	N	O	0	6	1
			317	205	55	57			
2	H	36	Total	C	N	O	0	3	1
			305	194	50	61			
2	J	37	Total	C	N	O	0	2	1
			299	192	51	56			
2	L	36	Total	C	N	O	0	2	1
			293	186	50	57			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	45	Total	O	0	1
			45	45		
3	C	40	Total	O	0	0
			40	40		
3	D	47	Total	O	0	3
			47	47		
3	E	37	Total	O	0	0
			37	37		
3	F	41	Total	O	0	1
			41	41		
3	G	26	Total	O	0	0
			26	26		
3	H	19	Total	O	0	0
			19	19		
3	I	27	Total	O	0	0
			27	27		
3	J	27	Total	O	0	1
			27	27		
3	K	33	Total	O	0	0
			33	33		
3	L	26	Total	O	0	0
			26	26		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.75Å 53.58Å 109.05Å 90.00° 94.96° 90.00°	Depositor
Resolution (Å)	48.01 – 1.85 48.01 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.01-1.85) 99.3 (48.01-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.180 , 0.240 0.189 , 0.248	Depositor DCC
R_{free} test set	1712 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4366	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.77% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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4.5 Carbohydrates [i](#)

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4.6 Ligand geometry [i](#)

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4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	42/44 (95%)	-0.43	0	100	100	13, 23, 33, 41	5 (11%)
1	C	42/44 (95%)	-0.45	0	100	100	13, 23, 33, 39	3 (7%)
1	E	42/44 (95%)	-0.25	0	100	100	12, 23, 36, 45	5 (11%)
1	G	42/44 (95%)	-0.07	0	100	100	15, 28, 35, 51	4 (9%)
1	I	42/44 (95%)	-0.00	1 (2%)	59	65	15, 27, 51, 70	4 (9%)
1	K	42/44 (95%)	-0.13	1 (2%)	59	65	15, 25, 32, 53	5 (11%)
2	B	33/37 (89%)	-0.17	1 (3%)	52	57	12, 25, 58, 73	7 (21%)
2	D	35/37 (94%)	-0.20	0	100	100	9, 26, 38, 60	4 (11%)
2	F	33/37 (89%)	-0.03	0	100	100	11, 25, 50, 54	6 (18%)
2	H	35/37 (94%)	0.41	1 (2%)	54	58	16, 38, 52, 66	3 (8%)
2	J	35/37 (94%)	0.48	1 (2%)	54	58	19, 39, 55, 73	2 (5%)
2	L	35/37 (94%)	0.47	4 (11%)	11	12	18, 36, 66, 75	2 (5%)
All	All	458/486 (94%)	-0.05	9 (1%)	64	71	9, 27, 52, 75	50 (10%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	452	ILE	4.4
1	K	184	ASN	3.6
2	B	454	LEU	3.3
2	L	454	LEU	3.1
2	L	453	SER	2.7
2	J	452	ILE	2.7
1	I	143	ASN	2.3
2	L	481	GLU	2.2
2	H	453	SER	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.