wwPDB X-ray Structure Validation Summary Report (i)

Feb 26, 2025 – 12:10 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 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 (i)) were used in the production of this report:

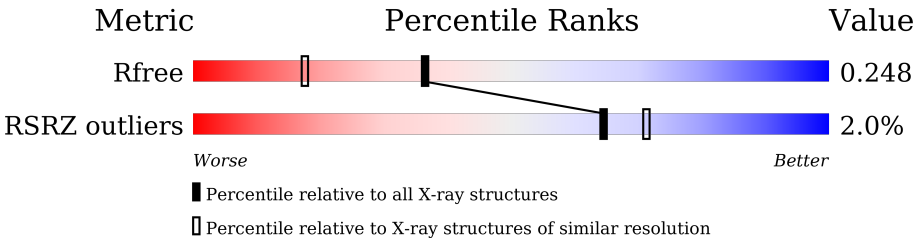
MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance (i)

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 (i)

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

- Molecule 3 is water.

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

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3 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

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

4.6 Ligand geometry

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

4.7 Other polymers

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

4.8 Polymer linkage issues (i)

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, 95^{th} 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%)

The worst 5 of 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

5.2 Non-standard residues in protein, DNA, RNA chains

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.