wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 06:38 AM EDT

PDB ID	:	6UJ9
Title	:	Crystal structure of HLA-B*07:02 with R140Q mutant IDH2 peptide in complex with Fab
Authors	:	Miller, M.S.; Thirawatananond, P.; Aytenfisu, T.Y.; Wright, K.; Gabelli, S.B.
Deposited on	:	2019-10-02
Resolution	:	2.90 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)	:	1.13
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)	:	2.35.1

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 2.90 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6557 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 HLA class I histocompatibility antigen, B-7 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2270	1409	415	439	7	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01889
A	281	GLY	-	expression tag	UNP P01889
A	282	SER	-	expression tag	UNP P01889
A	283	LEU	-	expression tag	UNP P01889
A	284	HIS	-	expression tag	UNP P01889
A	285	HIS	-	expression tag	UNP P01889
A	286	ILE	-	expression tag	UNP P01889
A	287	LEU	-	expression tag	UNP P01889
A	288	ASP	-	expression tag	UNP P01889
A	289	ALA	-	expression tag	UNP P01889
A	290	GLN	-	expression tag	UNP P01889
A	291	LYS	-	expression tag	UNP P01889
A	292	MET	-	expression tag	UNP P01889
A	293	VAL	-	expression tag	UNP P01889
A	294	TRP	-	expression tag	UNP P01889
A	295	ASN	-	expression tag	UNP P01889
A	296	HIS	-	expression tag	UNP P01889
A	297	ARG	-	expression tag	UNP P01889

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	834	531	141	159	3	0	0	0

- Molecule 3 is a protein called Isocitrate dehydrogenase [NADP], mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			74	45	13	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	7	GLN	ARG	engineered mutation	UNP P48735

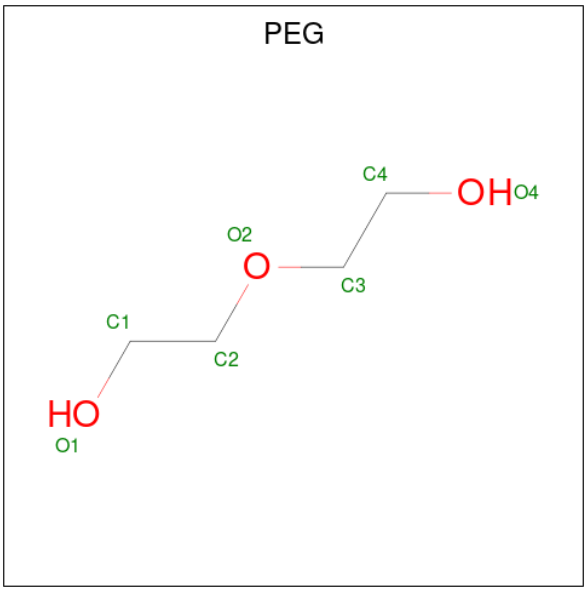
- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1642	1030	274	333	5			

- Molecule 5 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	218	Total	C	N	O	S	0	0	0
			1640	1040	272	321	7			

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

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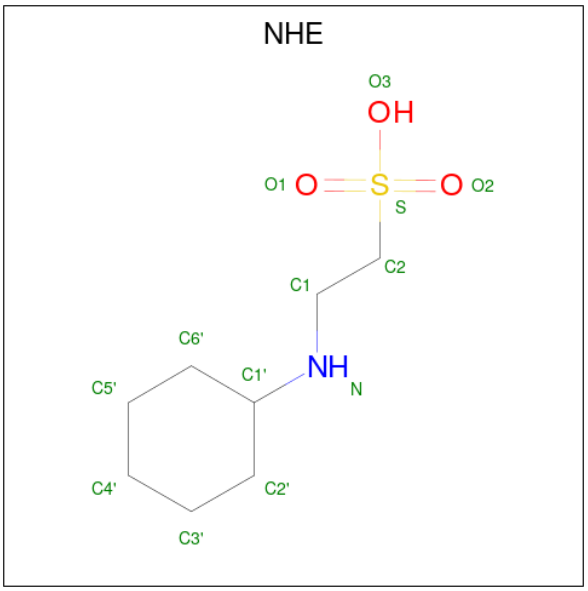
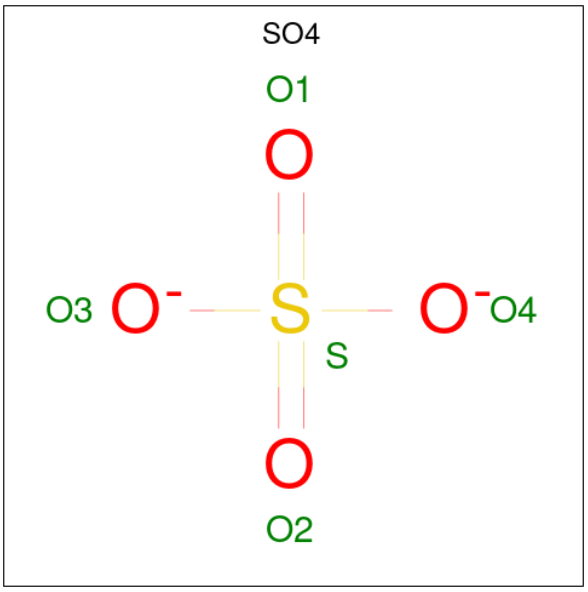
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	L	1	Total C O 7 4 3	0	0
6	L	1	Total C O 7 4 3	0	0

- Molecule 7 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O S 13 8 1 3 1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total O 1 1	0	0
9	H	1	Total O 1 1	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.61Å 42.01Å 125.18Å 90.00° 92.75° 90.00°	Depositor
Resolution (Å)	48.93 – 2.90	Depositor
% Data completeness (in resolution range)	98.2 (48.93-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.214 , 0.287	Depositor
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.396	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
Total number of atoms	6557	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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

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

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

15 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SO4	A	308	-	4,4,4	0.37	0	6,6,6	0.08	0
6	PEG	B	501	-	6,6,6	0.17	0	5,5,5	0.09	0
6	PEG	A	302	-	6,6,6	0.15	0	5,5,5	0.10	0
6	PEG	A	303	-	6,6,6	0.18	0	5,5,5	0.09	0
8	SO4	A	306	-	4,4,4	0.36	0	6,6,6	0.08	0
7	NHE	A	304	-	13,13,13	2.70	2 (15%)	16,17,17	2.62	7 (43%)
6	PEG	A	301	-	6,6,6	0.18	0	5,5,5	0.20	0
8	SO4	B	502	-	4,4,4	0.36	0	6,6,6	0.06	0
8	SO4	H	301	-	4,4,4	0.71	0	6,6,6	0.20	0
8	SO4	A	307	-	4,4,4	0.37	0	6,6,6	0.12	0
6	PEG	L	301	-	6,6,6	0.14	0	5,5,5	0.17	0
8	SO4	H	302	-	4,4,4	0.36	0	6,6,6	0.05	0
8	SO4	A	309	-	4,4,4	0.39	0	6,6,6	0.05	0
6	PEG	L	302	-	6,6,6	0.14	0	5,5,5	0.10	0
8	SO4	A	305	-	4,4,4	0.35	0	6,6,6	0.06	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
6	PEG	B	501	-	-	2/4/4/4	-
6	PEG	A	302	-	-	0/4/4/4	-
6	PEG	A	303	-	-	0/4/4/4	-
7	NHE	A	304	-	-	2/7/15/15	0/1/1/1
6	PEG	A	301	-	-	1/4/4/4	-
6	PEG	L	301	-	-	3/4/4/4	-
6	PEG	L	302	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	304	NHE	C2-S	-8.01	1.66	1.77
7	A	304	NHE	O3-S	5.18	1.65	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	304	NHE	C1-N-C1'	4.68	123.32	114.14
7	A	304	NHE	O3-S-C2	4.59	113.20	105.77
7	A	304	NHE	O1-S-C2	4.48	112.31	106.92
7	A	304	NHE	O2-S-C2	-3.78	102.36	106.92
7	A	304	NHE	C5'-C6'-C1'	3.58	117.84	111.11

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	304	NHE	N-C1-C2-S
6	L	301	PEG	O2-C3-C4-O4
6	L	301	PEG	O1-C1-C2-O2
7	A	304	NHE	C2-C1-N-C1'
6	B	501	PEG	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

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

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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