W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2017 – 06:26 PM EDT

PDB ID	:	3QEU
Title	:	The crystal structure of TCR DMF5
Authors	:	Borbulevych, O.Y.; Santhanagopolan, S.M.; Baker, B.M.
Deposited on	:	unknown
Resolution	:	2.09 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	**FAILED**
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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)	:	rb-20030345

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 2.09 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	Percentile Ranks	Value
Rfree		0.265
RSRZ outliers		15.9%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
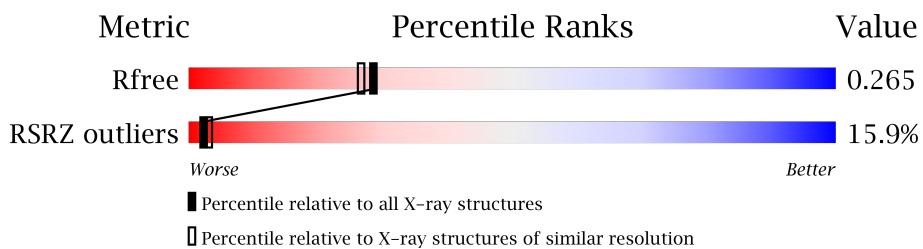
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4243 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7373 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 DMF5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	202	Total	C	N	O	S	0	2	0
			1573	982	258	325	8			
1	A	195	Total	C	N	O	S	0	1	0
			1516	947	249	312	8			

- Molecule 2 is a protein called DMF5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	243	Total	C	N	O	S	0	0	0
			1905	1196	334	366	9			
2	B	238	Total	C	N	O	S	0	0	0
			1868	1176	326	358	8			

- Molecule 3 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Li	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
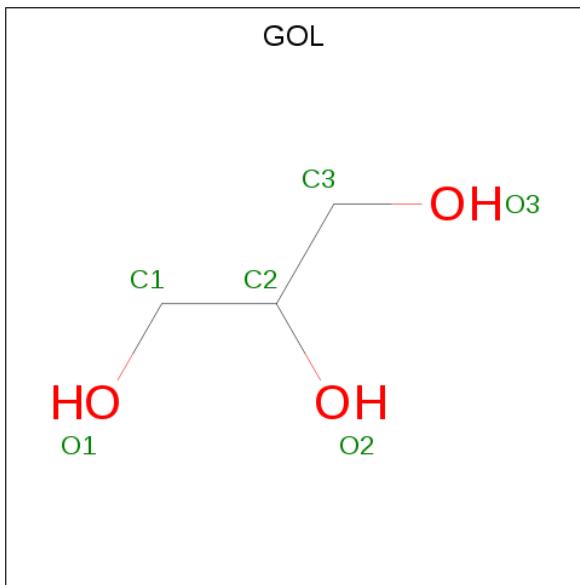
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	144	Total 144	O 144	0	0
5	E	208	Total 208	O 208	0	0
5	A	72	Total 72	O 72	0	0
5	B	74	Total 74	O 74	0	0

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3   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.16Å 86.50Å 66.47Å 90.00° 103.97° 90.00°	Depositor
Resolution (Å)	29.79 – 2.09 29.78 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.79-2.09) 99.1 (29.78-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.90 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.206 , 0.266 0.205 , 0.265	Depositor DCC
R_{free} test set	2977 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 64.1	EDS
L-test for twinning[2]	$<|L|> = 0.47$, $<L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7373	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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)

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

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

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

4.5 Carbohydrates (i)

There are no carbohydrates in this entry.

4.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	#$|Z| > 2$
4	GOL	B	246	-	5,5,5	0.13	0	5,5,5	1.14	0
4	GOL	E	2	-	5,5,5	0.35	0	5,5,5	0.31	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
4	GOL	B	246	-	-	0/4/4/4	0/0/0/0
4	GOL	E	2	-	-	0/4/4/4	0/0/0/0

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.

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 (i)

5.1 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(Å²)	Q<0.9
1	A	195/202 (96%)	1.62	59 (30%)	0	1	23, 45, 118, 119	0
1	D	202/202 (100%)	0.43	11 (5%)	26	33	14, 29, 45, 53	0
2	B	238/243 (97%)	1.23	59 (24%)	1	1	22, 54, 78, 90	0
2	E	243/243 (100%)	0.24	11 (4%)	34	40	17, 27, 47, 60	0
All	All	878/890 (98%)	0.86	140 (15%)	2	3	14, 35, 83, 119	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	TRP	13.9
1	A	188	ASN	9.0
1	A	189	SER	8.2
2	B	183	ALA	8.1
1	A	200	PRO	8.1
2	B	225	THR	7.5
1	A	146	SER	7.2
1	A	187	ASN	7.1
1	A	186	PHE	7.1
1	A	128	ASP	6.6
1	A	201	GLU	6.4
1	A	130	SER	6.3
1	A	127	SER	6.2
1	A	181	ALA	6.1
1	A	199	SER	6.1
1	A	126	SER	5.8
1	A	148	ASP	5.8
1	A	147	LYS	5.8
1	A	196	PHE	5.3
1	A	184	ASN	5.2
2	B	224	TRP	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	206	ARG	5.1
2	B	140	GLN	5.1
2	B	209	PHE	5.0
1	A	132	CYS	5.0
1	A	149	SER	4.9
1	D	128	ASP	4.8
1	A	122	ARG	4.7
1	A	124	SER	4.6
1	A	197	PHE	4.5
2	B	184	LEU	4.4
2	E	245	ASP	4.4
2	B	205	PRO	4.3
1	A	131	VAL	4.2
1	D	127	SER	4.1
2	B	137	SER	4.1
1	D	126	SER	4.1
1	A	94	GLY	4.1
2	B	219	SER	4.0
2	B	227	ASP	4.0
2	B	228	ARG	3.9
2	B	229	ALA	3.8
1	A	162	ARG	3.8
1	A	185	ALA	3.8
1	A	133	LEU	3.7
2	B	162	VAL	3.7
2	B	220	GLU	3.7
2	E	225	THR	3.5
2	B	119	ASN	3.5
1	A	182	CYS	3.4
2	B	222	ASP	3.4
2	B	223	GLU	3.4
1	A	163	SER	3.4
2	B	221	ASN	3.4
1	A	125	LYS	3.4
1	A	145	GLN	3.4
2	B	210	ARG	3.3
1	A	144	SER	3.3
1	D	50	TYR	3.3
2	B	185	ASN	3.3
2	B	164	GLY	3.3
1	A	113	ASN	3.2
2	E	223	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	198	PRO	3.2
2	B	147	LEU	3.2
2	B	117	ASP	3.1
2	B	230	LYS	3.1
1	A	193	GLU	3.1
2	B	138	HIS	3.1
2	E	42	LEU	3.1
2	E	227	ASP	3.0
1	A	129	LYS	3.0
2	E	3	MET	3.0
2	B	226	GLN	3.0
2	B	134	ALA	3.0
1	A	165	ASP	3.0
2	B	203	GLN	3.0
2	B	125	GLU	2.9
1	A	192	PRO	2.9
2	B	5	ALA	2.9
1	A	164	MET	2.9
2	B	100	PHE	2.9
1	A	190	ILE	2.9
2	B	143	THR	2.9
2	B	204	ASP	2.9
2	B	122	PHE	2.8
1	A	151	VAL	2.8
1	A	155	ASP	2.8
2	B	200	THR	2.8
2	B	182	PRO	2.8
2	B	44	LEU	2.8
2	B	116	GLU	2.8
2	B	133	GLU	2.8
2	E	185	ASN	2.8
1	D	94	GLY	2.8
2	E	220	GLU	2.7
2	B	195	LEU	2.7
2	B	126	VAL	2.7
1	A	28	GLY	2.7
2	B	130	GLU	2.7
1	A	26	ASP	2.7
2	B	168	HIS	2.6
2	B	42	LEU	2.6
2	B	201	PHE	2.6
1	A	150	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	118	VAL	2.5
2	B	86	PRO	2.5
1	D	27	ARG	2.5
1	A	1	LYS	2.5
2	B	16	LEU	2.5
2	B	136	ILE	2.5
2	E	100	PHE	2.5
2	B	124	PRO	2.5
2	E	221	ASN	2.5
1	A	152	TYR	2.5
2	E	145	VAL	2.4
1	D	201	GLU	2.4
1	A	120	GLN	2.4
1	A	191	ILE	2.4
2	B	118	LEU	2.4
2	B	115	VAL	2.4
2	B	241	TRP	2.4
1	A	183	ALA	2.3
2	B	161	TRP	2.3
1	D	0	ALA	2.3
1	A	195	THR	2.3
2	B	163	ASN	2.3
1	A	119	TYR	2.3
2	B	198	SER	2.3
2	B	145	VAL	2.3
1	D	93	GLY	2.2
1	D	179	ASP	2.2
1	A	116	PRO	2.2
1	A	158	VAL	2.2
1	A	134	PHE	2.1
2	B	4	ILE	2.1
1	D	171	ALA	2.0
1	A	135	THR	2.0
2	B	112	LEU	2.0
1	A	157	CYS	2.0

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 carbohydrates in this entry.

5.4 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(Å^2)	Q<0.9
4	GOL	B	246	6/6	0.83	0.20	1.62	34,40,41,41	0
4	GOL	E	2	6/6	0.88	0.23	-	53,54,54,55	6
3	LI	D	202	1/1	0.93	0.09	-	2,2,2,2	0

5.5 Other polymers (i)

There are no such residues in this entry.