WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2023 – 12:27 AM EDT

PDB ID	:	6VMJ
Title	:	Crystal structure of human Complement Factor D with anti-Factor D Fab 20D12
Authors	:	Wu, P.; Harris, S.F.; Eigenbrot, C.
Deposited on	:	2020-01-28
Resolution	:	2.95 Å(reported)

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 2.95 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.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	X	301	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19932 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 Fab20D12 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total 1635	C 1020	N 274	O 336	S 5	0	0	0
1	E	213	Total 1635	C 1020	N 274	O 336	S 5	0	0	0
1	I	213	Total 1635	C 1020	N 274	O 336	S 5	0	0	0
1	L	213	Total 1635	C 1020	N 274	O 336	S 5	0	0	0

- Molecule 2 is a protein called Fab20D12 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total 1574	C 997	N 257	O 315	S 5	0	0	0
2	F	211	Total 1574	C 997	N 257	O 315	S 5	0	0	0
2	J	211	Total 1574	C 997	N 257	O 315	S 5	0	0	0
2	M	213	Total 1589	C 1006	N 260	O 318	S 5	0	0	0

- Molecule 3 is a protein called Complement factor D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	228	Total 1713	C 1058	N 325	O 320	S 10	0	1	0
3	X	228	Total 1713	C 1058	N 325	O 320	S 10	0	1	0
3	Y	228	Total 1713	C 1058	N 325	O 320	S 10	0	1	0
3	Z	228	Total 1713	C 1058	N 325	O 320	S 10	0	1	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
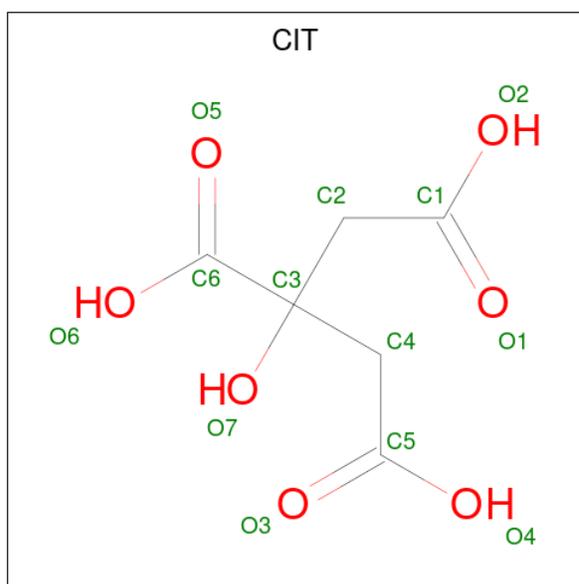
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 13	C 6	O 7	0	0
4	F	1	Total 13	C 6	O 7	0	0
4	J	1	Total 13	C 6	O 7	0	0
4	M	1	Total 13	C 6	O 7	0	0
4	W	1	Total 13	C 6	O 7	0	0
4	X	1	Total 13	C 6	O 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total 8	O 8	0	0
5	E	6	Total 6	O 6	0	0
5	F	6	Total 6	O 6	0	0
5	I	5	Total 5	O 5	0	0
5	J	15	Total 15	O 15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	21	Total 21	O 21	0	0
5	M	13	Total 13	O 13	0	0
5	W	23	Total 23	O 23	0	0
5	X	27	Total 27	O 27	0	0
5	Y	13	Total 13	O 13	0	0
5	Z	14	Total 14	O 14	0	0

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

3 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	180.84Å 180.84Å 304.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.24 – 2.95	Depositor
% Data completeness (in resolution range)	99.4 (47.24-2.95)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.217 , 0.265	Depositor
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.566	Xtriage
L-test for twinning[2]	$< |L| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19932	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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 ⓘ

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 ⓘ

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 ⓘ

6 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	$\#|Z| > 2$
4	CIT	X	301	-	12,12,12	1.87	5 (41%)	17,17,17	2.50	6 (35%)
4	CIT	J	301	-	12,12,12	0.52	0	17,17,17	0.85	1 (5%)
4	CIT	M	301	-	12,12,12	1.54	4 (33%)	17,17,17	2.33	5 (29%)
4	CIT	W	301	-	12,12,12	1.93	6 (50%)	17,17,17	2.41	6 (35%)
4	CIT	F	301	-	12,12,12	0.31	0	17,17,17	0.59	0
4	CIT	B	301	-	12,12,12	0.38	0	17,17,17	0.75	1 (5%)

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	CIT	X	301	-	-	7/16/16/16	-
4	CIT	J	301	-	-	2/16/16/16	-
4	CIT	M	301	-	-	6/16/16/16	-
4	CIT	W	301	-	-	2/16/16/16	-
4	CIT	F	301	-	-	0/16/16/16	-
4	CIT	B	301	-	-	0/16/16/16	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	301	CIT	O5-C6	3.16	1.32	1.22
4	X	301	CIT	O4-C5	-3.14	1.20	1.30
4	W	301	CIT	O3-C5	3.10	1.32	1.22
4	M	301	CIT	O5-C6	3.01	1.31	1.22
4	X	301	CIT	O5-C6	2.94	1.31	1.22

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	301	CIT	O5-C6-C3	-5.99	113.77	122.25
4	M	301	CIT	O5-C6-C3	-5.88	113.93	122.25
4	X	301	CIT	O5-C6-C3	-5.83	114.00	122.25
4	X	301	CIT	O6-C6-C3	5.52	122.63	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	301	CIT	O6-C6-C3	5.41	122.44	113.05

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	301	CIT	C2-C3-C6-O5
4	X	301	CIT	C2-C3-C6-O6
4	X	301	CIT	O7-C3-C6-O5
4	X	301	CIT	O7-C3-C6-O6
4	M	301	CIT	C2-C3-C6-O5

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers ⓘ

There are no such residues in this entry.

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 ⓘ

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.