



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:46 AM UTC

PDB ID : 5TBD / pdb_00005tbd
Title : Crystal Structure of anti-MSP2 Fv fragment (mAb4D11) in complex with 3D7-MSP2 215-222
Authors : Seow, J.; Morales, R.A.V.; MacRaild, C.A.; Bankala, K.; Drinkwater, N.; Dingjan, T.; Jaipuria, G.; Wilde, K.; Anders, R.F.; Atreya, H.S.; Christ, D.; McGowan, S.; Norton, R.S.
Deposited on : 2016-09-12
Resolution : 2.20 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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Mol	Chain	Length	Quality of chain
2	B	112	96%
2	F	112	88% 10%
2	G	112	2% 94% 5%
2	K	112	% 91% 8%
3	C	10	70% 30%
3	H	10	10% 90% 10%
3	I	10	80% 20%
3	L	10	80% 20%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7445 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 Fv fragment (mAb4D1) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	113	Total	C	N	O	S	0	0	0
			854	533	149	169	3			
1	A	114	Total	C	N	O	S	0	0	0
			868	540	151	174	3			
1	D	113	Total	C	N	O	S	0	0	0
			862	537	150	172	3			
1	J	113	Total	C	N	O	S	0	0	0
			853	531	149	170	3			

- Molecule 2 is a protein called Fv fragment (mAb4D1) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	111	Total	C	N	O	S	0	2	0
			859	547	141	168	3			
2	B	110	Total	C	N	O	S	0	0	0
			840	534	139	164	3			
2	G	112	Total	C	N	O	S	0	0	0
			851	542	140	166	3			
2	K	112	Total	C	N	O	S	0	2	0
			861	549	141	168	3			

- Molecule 3 is a protein called Merozoite surface protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	1
			58	32	12	13	1			
3	C	10	Total	C	N	O	S	0	0	1
			58	32	12	13	1			
3	H	10	Total	C	N	O	S	0	0	1
			58	32	12	13	1			
3	L	10	Total	C	N	O	S	0	0	1
			58	32	12	13	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	43	Total 43	O 43	0	0
4	F	56	Total 56	O 56	0	0
4	I	4	Total 4	O 4	0	0
4	A	40	Total 40	O 40	0	0
4	B	56	Total 56	O 56	0	0
4	C	1	Total 1	O 1	0	0
4	D	29	Total 29	O 29	0	0
4	G	63	Total 63	O 63	0	0
4	H	2	Total 2	O 2	0	0
4	J	19	Total 19	O 19	0	0
4	K	49	Total 49	O 49	0	0
4	L	3	Total 3	O 3	0	0

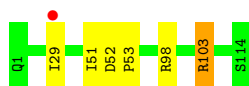
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

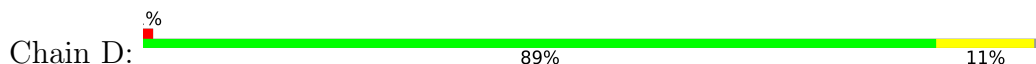
- Molecule 1: Fv fragment (mAb4D1) heavy chain



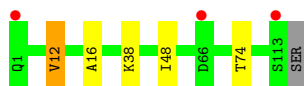
- Molecule 1: Fv fragment (mAb4D1) heavy chain



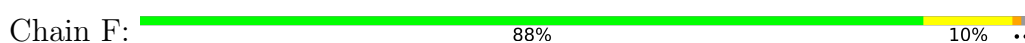
- Molecule 1: Fv fragment (mAb4D1) heavy chain



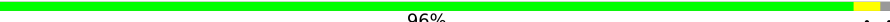
- Molecule 1: Fv fragment (mAb4D1) heavy chain



- Molecule 2: Fv fragment (mAb4D1) heavy chain



- Molecule 2: Fv fragment (mAb4D1) heavy chain

Chain B:  96% . .



- Molecule 2: Fv fragment (mAb4D1) heavy chain

Chain G:  94% 5% .



- Molecule 2: Fv fragment (mAb4D1) heavy chain

Chain K:  91% 8% .



- Molecule 3: Merozoite surface protein 2

Chain I:  80% 20%



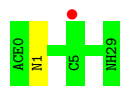
- Molecule 3: Merozoite surface protein 2

Chain C:  70% 30%



- Molecule 3: Merozoite surface protein 2

Chain H:  90% 10%



- Molecule 3: Merozoite surface protein 2

Chain L:  80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.98Å 72.97Å 81.97Å 68.19° 78.75° 73.83°	Depositor
Resolution (Å)	32.05 – 2.20 32.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.05-2.20) 100.0 (32.05-2.20)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.207 , 0.247 (Not available) , 0.238	Depositor DCC
R_{free} test set	2118 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7445	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, ACE

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/885	0.68	0/1204
1	D	0.25	0/879	0.65	0/1196
1	E	0.28	0/871	0.70	0/1186
1	J	0.25	0/870	0.68	0/1186
2	B	0.26	0/859	0.66	0/1167
2	F	0.26	0/881	0.63	0/1198
2	G	0.26	0/870	0.66	0/1183
2	K	0.26	0/886	0.66	0/1205
3	C	0.24	0/54	0.59	0/71
3	H	0.26	0/54	0.62	0/71
3	I	0.24	0/54	0.76	0/71
3	L	0.24	0/54	0.64	0/71
All	All	0.26	0/7217	0.67	0/9809

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	868	0	834	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	862	0	829	6	0
1	E	854	0	819	2	0
1	J	853	0	812	3	0
2	B	840	0	838	1	0
2	F	859	0	862	5	0
2	G	851	0	844	4	0
2	K	861	0	865	7	0
3	C	58	0	51	6	0
3	H	58	0	51	1	0
3	I	58	0	51	2	0
3	L	58	0	51	3	0
4	A	40	0	0	0	0
4	B	56	0	0	0	0
4	C	1	0	0	0	0
4	D	29	0	0	0	0
4	E	43	0	0	1	0
4	F	56	0	0	0	0
4	G	63	0	0	0	0
4	H	2	0	0	0	0
4	I	4	0	0	1	0
4	J	19	0	0	0	0
4	K	49	0	0	0	0
4	L	3	0	0	2	0
All	All	7445	0	6907	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:44:ARG:NH1	2:K:86:GLU:O	2.27	0.67
2:K:9:LEU:HD12	2:K:9:LEU:H	1.60	0.66
1:A:98:ARG:HH11	1:A:103:ARG:HH12	1.45	0.65
1:D:3:ARG:NH2	1:J:74:THR:O	2.31	0.64
1:A:52:ASP:OD1	3:C:2:LYS:NZ	2.30	0.64
3:I:2:LYS:NZ	4:I:101:HOH:O	2.35	0.58
2:K:66:ARG:NH2	2:K:87:ASP:OD2	2.37	0.57
3:C:0:ACE:H1	3:L:3:GLU:H	1.70	0.56
3:I:1:ASN:HA	3:H:1:ASN:HA	1.88	0.54
3:C:3:GLU:H	3:L:0:ACE:H1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:38:LEU:HD22	2:K:76:PHE:CG	2.45	0.51
1:D:47:TRP:HZ2	1:D:50:ARG:HB2	1.76	0.50
2:G:42:LEU:HD13	2:G:91:TYR:CZ	2.48	0.49
1:J:38:LYS:HB2	1:J:48:ILE:HD11	1.94	0.48
1:J:12:VAL:HG13	1:J:16:ALA:HB3	1.96	0.48
2:F:41:LEU:HD23	2:F:51:ARG:HA	1.95	0.48
1:D:73:ASP:HB3	1:D:76:SER:HB2	1.96	0.47
1:E:86:LEU:HD12	1:E:90:ASP:HB3	1.97	0.47
3:C:2:LYS:HG3	4:L:103:HOH:O	2.15	0.47
2:G:38:LEU:HD22	2:G:76:PHE:CG	2.50	0.47
1:E:1:GLN:N	4:E:205:HOH:O	2.46	0.46
2:K:1:ASP:OD1	2:K:1:ASP:N	2.35	0.46
1:D:60:TYR:HE2	1:D:70:ILE:HG13	1.82	0.45
2:F:70:SER:OG	2:F:77[A]:THR:OG1	2.34	0.44
1:D:91:THR:HG23	1:D:111:THR:HA	2.00	0.43
2:F:38:LEU:HD22	2:F:76:PHE:CG	2.54	0.43
2:G:38:LEU:HD22	2:G:76:PHE:CD2	2.53	0.42
3:C:0:ACE:H2	4:L:103:HOH:O	2.18	0.42
2:F:11:LEU:HD23	2:F:109:LEU:HD13	2.00	0.42
2:F:90:VAL:HG22	2:F:108:LYS:HD3	2.00	0.42
2:K:39:ASN:HB2	2:K:94:TRP:CE2	2.54	0.42
1:A:51:ILE:O	1:A:53:PRO:HD3	2.19	0.42
2:G:39:ASN:HB2	2:G:94:TRP:CE2	2.54	0.42
2:K:38:LEU:HG	2:K:39:ASN:N	2.34	0.41
3:C:0:ACE:CH3	3:L:3:GLU:H	2.34	0.41
1:D:18:VAL:HG22	1:D:86:LEU:HD11	2.03	0.41
2:B:63:VAL:HA	2:B:64:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/114 (92%)	104 (99%)	1 (1%)	0	100	100
1	D	45/114 (40%)	43 (96%)	2 (4%)	0	100	100
1	E	88/114 (77%)	85 (97%)	3 (3%)	0	100	100
1	J	111/114 (97%)	110 (99%)	1 (1%)	0	100	100
2	F	74/112 (66%)	72 (97%)	2 (3%)	0	100	100
2	G	93/112 (83%)	91 (98%)	2 (2%)	0	100	100
2	K	112/112 (100%)	109 (97%)	3 (3%)	0	100	100
3	H	8/10 (80%)	8 (100%)	0	0	100	100
3	L	8/10 (80%)	8 (100%)	0	0	100	100
All	All	644/812 (79%)	630 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/94 (98%)	90 (98%)	2 (2%)	45	61
1	D	91/94 (97%)	90 (99%)	1 (1%)	65	79
1	E	89/94 (95%)	89 (100%)	0	100	100
1	J	89/94 (95%)	88 (99%)	1 (1%)	65	79
2	B	97/99 (98%)	96 (99%)	1 (1%)	68	81
2	F	100/99 (101%)	97 (97%)	3 (3%)	36	49
2	G	97/99 (98%)	95 (98%)	2 (2%)	47	63
2	K	100/99 (101%)	99 (99%)	1 (1%)	68	81
3	C	5/5 (100%)	5 (100%)	0	100	100
3	H	5/5 (100%)	5 (100%)	0	100	100
3	I	5/5 (100%)	5 (100%)	0	100	100
3	L	5/5 (100%)	5 (100%)	0	100	100
All	All	775/792 (98%)	764 (99%)	11 (1%)	59	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	38	LEU
2	F	44	ARG
2	F	47	GLN
1	A	29	ILE
1	A	103	ARG
2	B	38	LEU
1	D	11	LEU
2	G	13	VAL
2	G	38	LEU
1	J	12	VAL
2	K	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	17	GLN
2	F	27	GLN
1	J	5	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 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	114/114 (100%)	0.26	1 (0%) 81 79	14, 25, 44, 66	0
1	D	113/114 (99%)	0.19	1 (0%) 81 79	15, 26, 41, 54	0
1	E	113/114 (99%)	0.53	13 (11%) 9 7	16, 27, 58, 79	0
1	J	113/114 (99%)	0.51	3 (2%) 56 53	17, 31, 58, 73	0
2	B	110/112 (98%)	0.05	0 100 100	14, 23, 38, 49	0
2	F	111/112 (99%)	0.00	0 100 100	8, 19, 36, 41	2 (1%)
2	G	112/112 (100%)	0.04	2 (1%) 67 64	14, 24, 37, 67	0
2	K	112/112 (100%)	0.27	1 (0%) 81 79	13, 27, 40, 54	2 (1%)
3	C	8/10 (80%)	-0.10	0 100 100	16, 18, 20, 21	0
3	H	8/10 (80%)	0.22	1 (12%) 8 6	18, 21, 24, 29	0
3	I	8/10 (80%)	0.03	0 100 100	15, 18, 24, 25	0
3	L	8/10 (80%)	-0.16	0 100 100	15, 18, 22, 23	0
All	All	930/944 (98%)	0.23	22 (2%) 59 56	8, 25, 47, 79	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	89	GLU	4.2
1	E	15	GLY	3.6
1	E	17	SER	3.5
1	E	112	VAL	3.4
1	E	16	ALA	3.2
2	K	99	PHE	3.2
1	E	84	THR	3.0
1	E	113	SER	3.0
1	J	1	GLN	2.8
2	G	112	LYS	2.7
2	G	111	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	56	GLY	2.5
1	E	11	LEU	2.4
1	E	13	LYS	2.3
1	E	12	VAL	2.3
1	E	66	ASP	2.3
1	E	65	GLN	2.2
1	J	66	ASP	2.2
1	J	113	SER	2.2
3	H	5	CYS	2.1
1	A	29	ILE	2.1
1	E	85	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.