



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:37 am GMT

PDB ID : 4HS6
Title : Hepatitis C envelope glycoprotein E2 fragment 412-423 with humanized and affinity-matured antibody MRCT10.v362
Authors : Eigenbrot, C.; Ultsch, M.
Deposited on : 2012-10-29
Resolution : 1.53 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

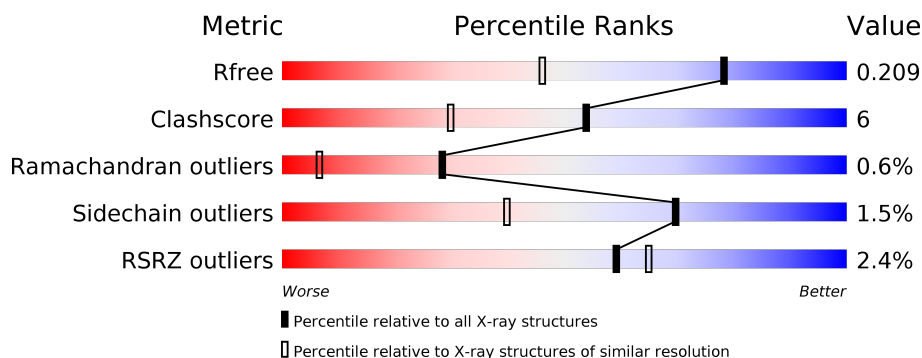
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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}	100719	1773 (1.56-1.52)
Clashscore	112137	1845 (1.56-1.52)
Ramachandran outliers	110173	1810 (1.56-1.52)
Sidechain outliers	110143	1808 (1.56-1.52)
RSRZ outliers	101464	1774 (1.56-1.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Y	16	<div> <div>13%</div> <div> <div></div> <div>50%</div> <div>25%</div> <div>25%</div> </div> </div>
1	Z	16	<div> <div>6%</div> <div> <div></div> <div>56%</div> <div>19%</div> <div>25%</div> </div> </div>
2	A	218	<div> <div></div> <div> <div></div> <div>87%</div> <div>11%</div> <div>•</div> </div> </div>
2	L	218	<div> <div>•</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
3	B	226	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>•</div> <div>5%</div> </div> </div>
3	H	226	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7966 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 E2-peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Z	12	Total	C	N	O	0	1	0
			105	66	21	18			
1	Y	12	Total	C	N	O	0	0	0
			98	61	19	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	424	GLY	-	EXPRESSION TAG	UNP Q9YK84
Z	425	SER	-	EXPRESSION TAG	UNP Q9YK84
Z	426	GLY	-	EXPRESSION TAG	UNP Q9YK84
Z	427	LYS	-	EXPRESSION TAG	UNP Q9YK84
Y	424	GLY	-	EXPRESSION TAG	UNP Q9YK84
Y	425	SER	-	EXPRESSION TAG	UNP Q9YK84
Y	426	GLY	-	EXPRESSION TAG	UNP Q9YK84
Y	427	LYS	-	EXPRESSION TAG	UNP Q9YK84

- Molecule 2 is a protein called MRCT10.v362 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	218	Total	C	N	O	S	19	7	0
			1720	1082	286	346	6			
2	L	218	Total	C	N	O	S	19	5	0
			1703	1069	284	344	6			

- Molecule 3 is a protein called MRCT10.v362 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	214	Total	C	N	O	S	0	6	0
			1639	1039	263	329	8			
3	H	215	Total	C	N	O	S	0	4	0
			1642	1036	268	330	8			

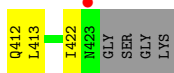
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Z	15	Total 15	O 15	0	0
4	Y	14	Total 14	O 14	0	0
4	A	225	Total 225	O 225	0	0
4	L	252	Total 252	O 252	0	0
4	B	276	Total 276	O 276	0	0
4	H	277	Total 277	O 277	0	0

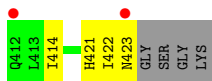
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: E2-peptide



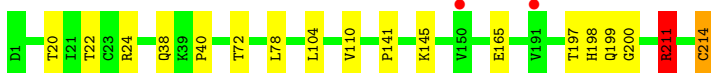
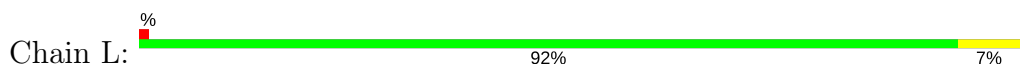
- Molecule 1: E2-peptide



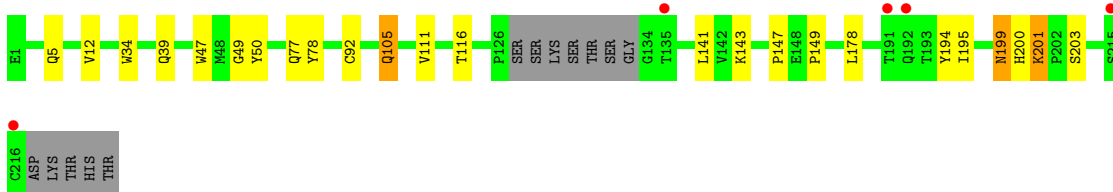
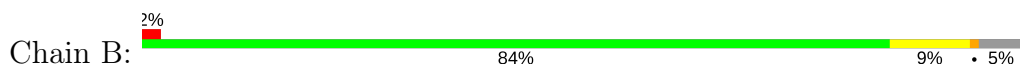
- Molecule 2: MRCT10.v362 Fab light chain



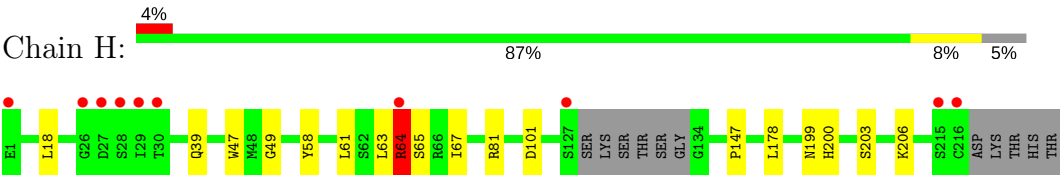
- Molecule 2: MRCT10.v362 Fab light chain



- Molecule 3: MRCT10.v362 Fab heavy chain



● Molecule 3: MRCT10.v362 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.09Å 90.82Å 72.68Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	50.00 – 1.53 37.79 – 1.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.53) 99.9 (37.79-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.200 0.186 , 0.209	Depositor DCC
R_{free} test set	1318 reflections (1.02%)	DCC
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7966	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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

5.1 Standard geometry

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	Y	0.37	0/100	0.46	0/136
1	Z	0.39	0/111	0.51	0/151
2	A	0.91	2/1776 (0.1%)	0.62	0/2410
2	L	0.50	2/1756 (0.1%)	0.65	2/2384 (0.1%)
3	B	0.44	0/1696	0.63	0/2320
3	H	0.41	0/1690	0.62	0/2309
All	All	0.60	4/7129 (0.1%)	0.63	2/9710 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1
2	L	0	1
3	H	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	214	CYS	CB-SG	33.04	2.38	1.82
2	L	211	ARG	C-N	11.59	1.53	1.33
2	A	211	ARG	C-N	8.79	1.48	1.33
2	L	214	CYS	CB-SG	5.70	1.92	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	211	ARG	CA-C-N	-11.24	93.72	116.20
2	L	211	ARG	C-N-CA	-5.36	111.04	122.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	211	ARG	Mainchain
3	H	63	LEU	Peptide
2	L	211	ARG	Mainchain

5.2 Too-close contacts

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	Y	98	0	90	2	0
1	Z	105	0	97	3	0
2	A	1720	0	1681	22	0
2	L	1703	0	1656	24	0
3	B	1639	0	1626	21	0
3	H	1642	0	1617	15	0
4	A	225	0	0	5	0
4	B	276	0	0	3	0
4	H	277	0	0	1	0
4	L	252	0	0	0	0
4	Y	14	0	0	1	0
4	Z	15	0	0	0	0
All	All	7966	0	6767	83	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 6.

The worst 5 of 83 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:L:24[B]:ARG:HG2	2:L:24[B]:ARG:HH21	1.05	1.14
2:L:24[B]:ARG:CG	2:L:24[B]:ARG:HH21	1.80	0.95
2:A:38:GLN:HE22	3:B:39:GLN:HE22	1.16	0.88
2:L:24[B]:ARG:NH2	2:L:24[B]:ARG:HG2	1.87	0.82
3:B:105:GLN:CD	3:B:105:GLN:H	1.89	0.75

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	Y	10/16 (62%)	10 (100%)	0	0	100	100
1	Z	11/16 (69%)	11 (100%)	0	0	100	100
2	A	223/218 (102%)	217 (97%)	5 (2%)	1 (0%)	38	14
2	L	221/218 (101%)	216 (98%)	4 (2%)	1 (0%)	32	9
3	B	215/226 (95%)	208 (97%)	6 (3%)	1 (0%)	32	9
3	H	215/226 (95%)	209 (97%)	4 (2%)	2 (1%)	20	3
All	All	895/920 (97%)	871 (97%)	19 (2%)	5 (1%)	28	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	211	ARG
3	H	64	ARG
2	L	211	ARG
3	B	149	PRO
3	H	65	SER

5.3.2 Protein sidechains [i](#)

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	Y	11/13 (85%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	12/13 (92%)	12 (100%)	0	100	100
2	A	199/192 (104%)	193 (97%)	6 (3%)	46	14
2	L	197/192 (103%)	196 (100%)	1 (0%)	91	79
3	B	192/197 (98%)	188 (98%)	4 (2%)	59	26
3	H	191/197 (97%)	189 (99%)	2 (1%)	80	59
All	All	802/804 (100%)	789 (98%)	13 (2%)	70	37

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	214	CYS
2	L	214	CYS
3	B	201	LYS
2	A	147	GLN
3	B	199	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	198	HIS
2	L	199	GLN
3	H	5	GLN
2	L	53	ASN
3	B	200	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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 [i](#)

6.1 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(Å ²)	Q<0.9
1	Y	12/16 (75%)	0.50	2 (16%) 2 1	17, 21, 45, 59	0
1	Z	12/16 (75%)	0.43	1 (8%) 12 14	15, 23, 37, 62	0
2	A	216/218 (99%)	-0.14	1 (0%) 90 92	12, 22, 42, 82	1 (0%)
2	L	216/218 (99%)	-0.12	2 (0%) 84 86	14, 23, 40, 82	1 (0%)
3	B	214/226 (94%)	-0.14	5 (2%) 61 66	12, 19, 39, 91	1 (0%)
3	H	215/226 (95%)	-0.04	10 (4%) 32 36	12, 18, 38, 76	2 (0%)
All	All	885/920 (96%)	-0.09	21 (2%) 59 65	12, 21, 40, 91	5 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	215	SER	8.4
3	H	216	CYS	6.8
1	Y	423	ASN	4.5
1	Z	423	ASN	4.3
3	H	215	SER	4.2

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 carbohydrates 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.