Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 09:20 pm GMT

PDB ID	:	8CHE
Title	:	TLT-1 binding Fab of the bispecific antibody HMB-001 in complex with the TLT-1 stalk peptide
Authors	:	Johansson, E.; Schluckebier, G.
Deposited on	:	2023-02-07
Resolution	:	1.49 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:

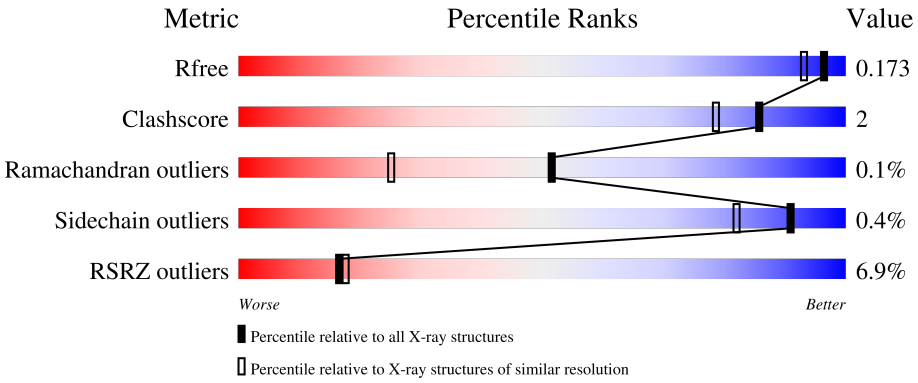
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.49 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.



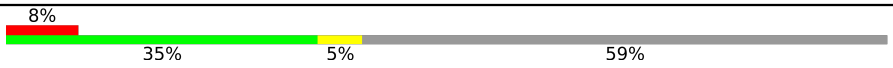
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	A	215	5% 97% .
1	H	215	5% 97% .
2	B	219	7% 98% .
2	L	219	10% 91% 9%
3	C	37	5% 38% . 59%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	37	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14866 atoms, of which 6832 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 Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	214	Total	C	H	N	O	S	0	14	0
			3304	1045	1634	281	336	8			
1	A	214	Total	C	H	N	O	S	0	10	0
			3264	1032	1613	279	332	8			

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	219	Total	C	H	N	O	S	0	9	0
			3442	1086	1697	302	349	8			
2	B	219	Total	C	H	N	O	S	0	6	0
			3419	1080	1686	300	345	8			

- Molecule 3 is a protein called Trem-like transcript 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	H	N	O	0	0	0
			210	68	101	19	22			
3	D	15	Total	C	H	N	O	0	0	0
			210	68	101	19	22			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	261	Total	O	0	0
			261	261		
4	L	227	Total	O	0	0
			227	227		
4	A	275	Total	O	0	0
			275	275		
4	B	215	Total	O	0	0
			215	215		

Continued on next page...

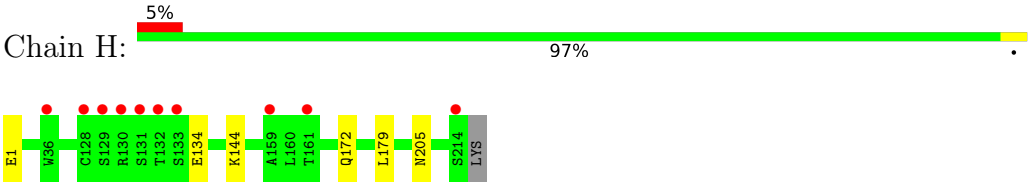
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	21	Total O 21 21	0	0
4	D	18	Total O 18 18	0	0

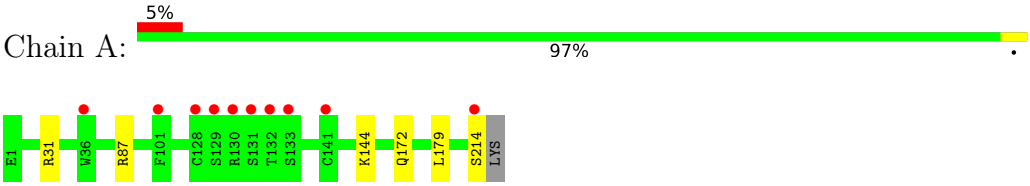
3 Residue-property plots (i)

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.

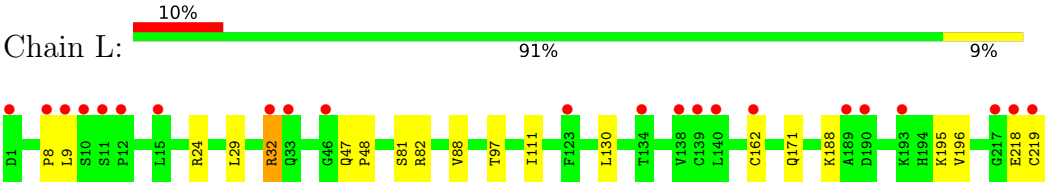
• Molecule 1: Fab heavy chain



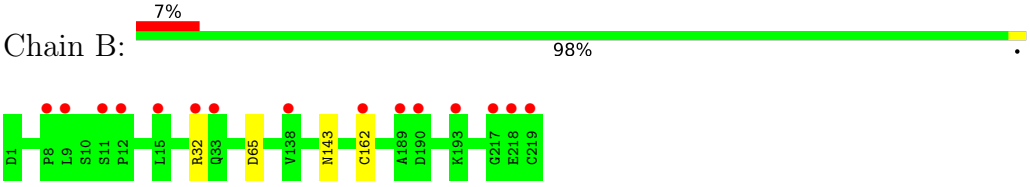
• Molecule 1: Fab heavy chain



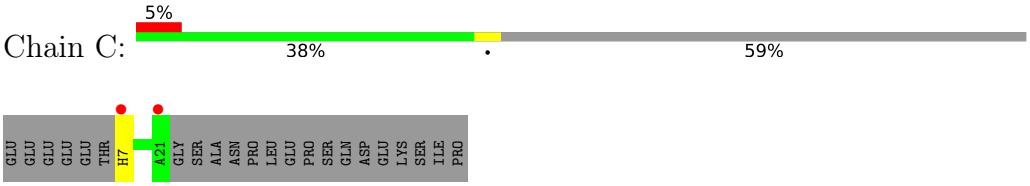
• Molecule 2: Fab light chain



• Molecule 2: Fab light chain

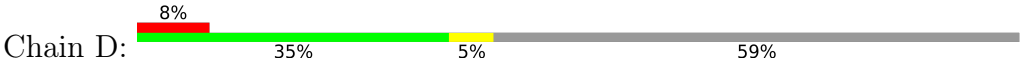


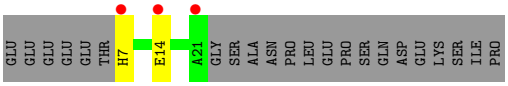
• Molecule 3: Trem-like transcript 1 protein



• Molecule 3: Trem-like transcript 1 protein

Chain D:


8%
35%
5%
59%


GLU
GLU
GLU
GLU
GLU
THR
H7
E14
A21
GLY
SER
ALA
ASN
PRO
LEU
GLU
PRO
SER
GLN
ASP
GLU
LYS
SER
ILE
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.23Å 65.38Å 67.14Å 91.88° 91.72° 92.89°	Depositor
Resolution (Å)	28.46 – 1.49 28.47 – 1.49	Depositor EDS
% Data completeness (in resolution range)	91.0 (28.46-1.49) 91.0 (28.47-1.49)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.49Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.157 , 0.174 0.156 , 0.173	Depositor DCC
R_{free} test set	1783 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14866	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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.

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	A	0.54	0/1698	0.71	0/2315
1	H	0.51	0/1723	0.69	0/2352
2	B	0.49	0/1781	0.66	0/2417
2	L	0.45	0/1802	0.64	0/2445
3	C	0.38	0/111	0.42	0/149
3	D	0.43	0/111	0.49	0/149
All	All	0.49	0/7226	0.67	0/9827

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

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	1651	1613	1591	5	0
1	H	1670	1634	1592	5	0
2	B	1733	1686	1675	5	0
2	L	1745	1697	1676	14	0
3	C	109	101	101	1	0
3	D	109	101	101	1	0
4	A	275	0	0	4	3
4	B	215	0	0	1	3
4	C	21	0	0	1	0
4	D	18	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	261	0	0	2	4
4	L	227	0	0	4	3
All	All	8034	6832	6736	30	7

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 2.

All (30) 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:B:162:CYS:SG	4:B:493:HOH:O	2.10	1.07
1:A:87:ARG:NH2	4:A:301:HOH:O	2.01	0.93
2:L:162:CYS:SG	4:L:518:HOH:O	2.36	0.83
1:H:205:ASN:ND2	4:H:301:HOH:O	2.26	0.69
2:L:29:LEU:O	2:L:97[A]:THR:HG21	1.94	0.68
2:L:82:ARG:NH2	2:B:65:ASP:OD2	2.27	0.67
2:L:32:ARG:O	4:L:302:HOH:O	2.14	0.64
2:L:81[A]:SER:O	4:L:301:HOH:O	2.10	0.63
3:D:14:GLU:OE1	4:D:101:HOH:O	2.15	0.63
2:L:81[B]:SER:O	4:L:301:HOH:O	2.16	0.58
1:H:144:LYS:NZ	1:H:172:GLN:OE1	2.38	0.57
1:A:31:ARG:NH1	4:A:306:HOH:O	2.34	0.57
2:L:195:LYS:HE2	2:L:196:VAL:CG2	2.37	0.55
1:H:134:GLU:CG	4:H:310:HOH:O	2.55	0.54
3:C:7:HIS:N	4:C:101:HOH:O	2.44	0.49
2:L:88:VAL:HB	2:L:111:ILE:HD13	1.94	0.49
2:B:32:ARG:CZ	2:B:32:ARG:H	2.28	0.46
1:H:179:LEU:C	1:H:179:LEU:HD12	2.37	0.45
2:L:130:LEU:O	2:L:188:LYS:HD3	2.16	0.45
1:A:214:SER:HB2	4:A:542:HOH:O	2.19	0.43
1:A:144:LYS:NZ	1:A:172:GLN:OE1	2.51	0.43
1:A:179:LEU:HD12	1:A:179:LEU:C	2.39	0.43
2:L:8:PRO:O	2:L:9:LEU:HD12	2.19	0.43
2:L:47:GLN:HE21	2:L:48:PRO:HD2	1.85	0.41
2:L:88:VAL:HG21	2:L:171:GLN:HB3	2.03	0.41
2:B:32:ARG:NE	2:B:32:ARG:HA	2.36	0.41
1:H:1[B]:GLU:HG2	2:B:143:ASN:ND2	2.35	0.41
2:L:24:ARG:HB3	2:L:24:ARG:NH1	2.37	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:513:HOH:O	4:B:438:HOH:O[1_455]	1.82	0.38
4:H:478:HOH:O	4:L:425:HOH:O[1_455]	1.97	0.23
4:A:538:HOH:O	4:B:485:HOH:O[1_554]	2.06	0.14
4:H:303:HOH:O	4:A:504:HOH:O[1_565]	2.09	0.11
4:H:327:HOH:O	4:L:367:HOH:O[1_455]	2.15	0.05
4:B:472:HOH:O	4:B:500:HOH:O[1_455]	2.16	0.04
4:H:503:HOH:O	4:L:378:HOH:O[1_455]	2.19	0.01

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	A	222/215 (103%)	217 (98%)	5 (2%)	0	100 100
1	H	224/215 (104%)	219 (98%)	5 (2%)	0	100 100
2	B	223/219 (102%)	217 (97%)	6 (3%)	0	100 100
2	L	226/219 (103%)	218 (96%)	7 (3%)	1 (0%)	34 13
3	C	13/37 (35%)	13 (100%)	0	0	100 100
3	D	13/37 (35%)	13 (100%)	0	0	100 100
All	All	921/942 (98%)	897 (97%)	23 (2%)	1 (0%)	51 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	32	ARG

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	A	191/182 (105%)	191 (100%)	0	100 100
1	H	194/182 (107%)	194 (100%)	0	100 100
2	B	202/196 (103%)	202 (100%)	0	100 100
2	L	205/196 (105%)	203 (99%)	2 (1%)	76 57
3	C	11/31 (36%)	11 (100%)	0	100 100
3	D	11/31 (36%)	10 (91%)	1 (9%)	9 0
All	All	814/818 (100%)	811 (100%)	3 (0%)	91 82

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	218	GLU
2	L	219	CYS
3	D	7	HIS

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

Mol	Chain	Res	Type
1	H	205	ASN
2	L	47	GLN
2	B	47	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	214/215 (99%)	0.20	10 (4%) 31 34	12, 17, 37, 123	0
1	H	214/215 (99%)	0.17	10 (4%) 31 34	14, 18, 37, 60	0
2	B	219/219 (100%)	0.23	15 (6%) 17 18	14, 20, 38, 73	0
2	L	219/219 (100%)	0.40	22 (10%) 7 7	15, 22, 42, 109	0
3	C	15/37 (40%)	0.54	2 (13%) 3 3	18, 22, 47, 85	0
3	D	15/37 (40%)	0.73	3 (20%) 1 1	16, 19, 42, 74	0
All	All	896/942 (95%)	0.26	62 (6%) 16 17	12, 19, 40, 123	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	7	HIS	8.5
1	A	130	ARG	7.4
2	L	219	CYS	6.8
2	B	219	CYS	6.8
3	C	7	HIS	6.4
2	L	32	ARG	6.2
2	L	33	GLN	5.9
2	L	217	GLY	5.8
1	A	131	SER	5.6
2	B	162	CYS	5.5
1	A	129	SER	5.3
2	L	162	CYS	5.2
2	B	33	GLN	5.0
2	B	32	ARG	4.7
2	L	9	LEU	4.6
1	A	132	THR	4.3
1	H	214	SER	4.1
2	L	11	SER	4.1
1	A	128	CYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	129	SER	3.9
2	B	9	LEU	3.8
2	B	218	GLU	3.8
2	L	8	PRO	3.6
1	A	214	SER	3.5
3	C	21	ALA	3.5
1	A	133	SER	3.5
1	H	131	SER	3.3
2	B	217	GLY	3.3
1	H	132	THR	3.2
1	H	128	CYS	3.2
2	L	218	GLU	3.1
2	L	138	VAL	3.0
2	B	8	PRO	3.0
1	A	36	TRP	3.0
1	H	130	ARG	2.8
1	A	101	PHE	2.7
2	L	123	PHE	2.7
1	H	36	TRP	2.6
2	L	46	GLY	2.6
2	L	1	ASP	2.6
1	H	133	SER	2.6
2	L	189	ALA	2.5
2	L	134	THR	2.5
3	D	14	GLU	2.4
2	L	140	LEU	2.4
3	D	21	ALA	2.4
2	B	190	ASP	2.4
2	B	11	SER	2.3
2	B	15	LEU	2.3
1	H	161	THR	2.2
1	A	141[A]	CYS	2.2
2	L	10	SER	2.2
1	H	159	ALA	2.2
2	B	12	PRO	2.2
2	L	193	LYS	2.2
2	L	190	ASP	2.1
2	L	139	CYS	2.1
2	L	15	LEU	2.1
2	B	193	LYS	2.1
2	B	138	VAL	2.1
2	B	189	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	12	PRO	2.0

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 monosaccharides 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.