Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2022 – 03:25 pm GMT

PDB ID	:	6TKB
Title	:	ChiLob 7/4 H2 HC-C224S F(ab')2
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Deposited on	:	2019-11-28
Resolution	:	2.00 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:

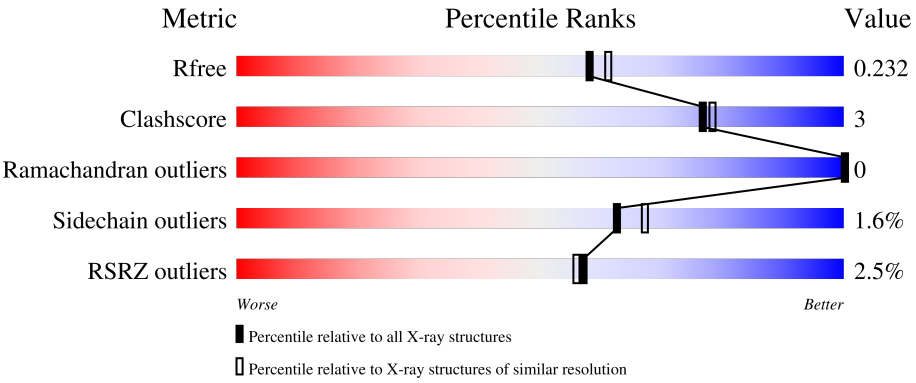
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	HHH	231	2% 93% 5% ·
1	III	231	5% 88% 8% ·
2	LLL	214	92% 8%
2	MMM	214	3% 85% 14% ·

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13668 atoms, of which 6502 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 Chilob 7/4 H2 heavy chain C224S.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HHH	227	Total	C	H	N	O	S	109	0	0
			3420	1088	1687	288	348	9			
1	III	221	Total	C	H	N	O	S	105	0	0
			3304	1047	1632	278	338	9			

- Molecule 2 is a protein called Chilob 7/4 H2 kappa chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	LLL	214	Total	C	H	N	O	S	118	1	0
			3249	1031	1594	273	345	6			
2	MMM	214	Total	C	H	N	O	S	117	0	0
			3238	1028	1589	272	343	6			

- Molecule 3 is water.

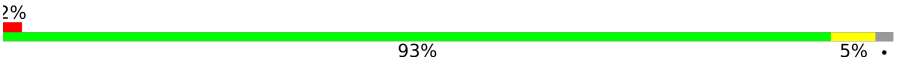
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	HHH	166	Total	O	0	0
			166	166		
3	LLL	137	Total	O	0	0
			137	137		
3	III	112	Total	O	0	0
			112	112		
3	MMM	42	Total	O	0	0
			42	42		

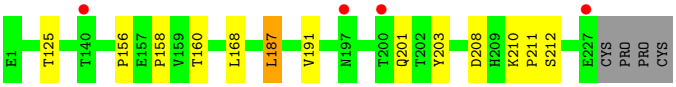
3 Residue-property plots (i)

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: Chilob 7/4 H2 heavy chain C224S

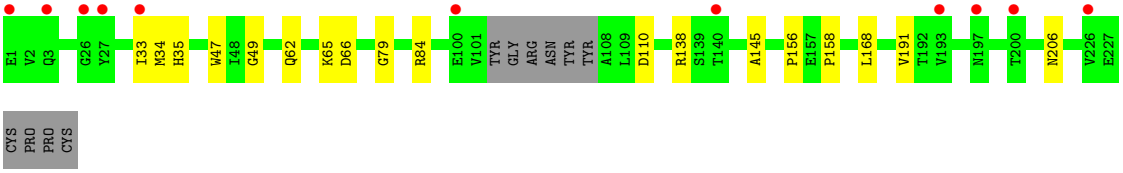
Chain HHH:





• Molecule 1: Chilob 7/4 H2 heavy chain C224S

Chain III:



• Molecule 2: Chilob 7/4 H2 kappa chain

Chain LLL:

• Molecule 2: Chilob 7/4 H2 kappa chain

Chain MMM:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.76Å 95.19Å 150.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 2.00 47.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.64-2.00) 99.7 (47.60-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.182 , 0.229 0.190 , 0.232	Depositor DCC
R_{free} test set	3619 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13668	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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	HHH	0.73	0/1774	0.87	0/2413
1	III	0.76	0/1709	0.86	0/2323
2	LLL	0.72	0/1689	0.92	2/2294 (0.1%)
2	MMM	0.71	0/1683	0.86	0/2286
All	All	0.73	0/6855	0.88	2/9316 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	LLL	96	TYR	CB-CG-CD1	6.62	124.97	121.00
2	LLL	96	TYR	CB-CG-CD2	-6.43	117.14	121.00

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	HHH	1733	1687	1683	7	0
1	III	1672	1632	1626	9	0
2	LLL	1655	1594	1590	8	0
2	MMM	1649	1589	1586	16	0
3	HHH	166	0	0	0	0
3	III	112	0	0	0	0
3	LLL	137	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	MMM	42	0	0	0	0
All	All	7166	6502	6485	39	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 (39) 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)
1:III:168:LEU:HD21	1:III:191:VAL:HG11	1.81	0.63
2:MMM:40:PRO:HB3	2:MMM:165:GLU:HG3	1.83	0.60
2:MMM:31:ASN:ND2	2:MMM:66:GLY:O	2.40	0.55
1:III:34:MET:SD	1:III:79:GLY:HA3	2.46	0.55
2:MMM:140:TYR:CG	2:MMM:141:PRO:HA	2.42	0.54
2:LLL:40:PRO:HB3	2:LLL:165:GLU:HG3	1.89	0.53
1:III:66:ASP:HA	1:III:84:ARG:NH2	2.24	0.53
1:III:138:ARG:HE	1:III:145:ALA:HB1	1.74	0.52
2:MMM:11:LEU:HD11	2:MMM:104:LEU:HD13	1.92	0.52
2:MMM:78:LEU:HD11	2:MMM:104:LEU:HD21	1.93	0.51
2:LLL:142:ARG:NH1	2:LLL:163:VAL:HG11	2.25	0.51
1:HHH:187:LEU:C	1:HHH:187:LEU:HD12	2.30	0.51
2:MMM:19:VAL:O	2:MMM:74:THR:HA	2.11	0.51
2:MMM:186:TYR:CE2	2:MMM:211:ARG:HD2	2.46	0.50
1:III:62:GLN:OE1	1:III:65:LYS:HE3	2.11	0.49
2:MMM:12:SER:HA	2:MMM:105:GLU:O	2.14	0.48
1:HHH:160:THR:OG1	1:HHH:208:ASP:HB3	2.14	0.47
1:HHH:125:THR:HG22	1:HHH:212:SER:HB3	1.96	0.47
2:MMM:16:GLY:HA2	2:MMM:77:ASN:HA	1.97	0.47
1:HHH:201:GLN:HG3	1:HHH:203:TYR:CZ	2.50	0.46
2:LLL:105:GLU:HG2	2:LLL:106:ILE:N	2.30	0.46
1:HHH:168:LEU:HD21	1:HHH:191:VAL:HG11	1.98	0.45
1:HHH:210:LYS:N	1:HHH:211:PRO:CD	2.79	0.45
2:LLL:80:PRO:HB2	2:LLL:168:SER:O	2.17	0.45
2:MMM:40:PRO:HB3	2:MMM:165:GLU:CG	2.47	0.45
1:III:138:ARG:NE	1:III:145:ALA:HB1	2.33	0.44
2:MMM:145:LYS:HB3	2:MMM:197:THR:HB	1.99	0.44
2:LLL:18:ARG:HG3	2:LLL:76:SER:HA	1.99	0.44
1:III:47:TRP:CZ2	1:III:49:GLY:HA2	2.53	0.44
2:MMM:80:PRO:HA	2:MMM:106:ILE:HD13	2.00	0.43
2:LLL:39:LYS:HE2	2:LLL:81:GLU:O	2.18	0.43
2:MMM:163:VAL:HG22	2:MMM:175:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:MMM:4:MET:HE2	2:MMM:23:CYS:SG	2.61	0.41
1:HHH:125:THR:CG2	1:HHH:212:SER:HB3	2.51	0.41
2:MMM:192:TYR:O	2:MMM:208:SER:HA	2.21	0.41
2:LLL:159:SER:HA	2:LLL:178:THR:O	2.21	0.40
1:III:33:ILE:HG22	1:III:35:HIS:CD2	2.56	0.40
2:LLL:192:TYR:O	2:LLL:208:SER:HA	2.21	0.40
1:III:110:ASP:HA	2:MMM:46:LEU:HD22	2.02	0.40

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	HHH	225/231 (97%)	222 (99%)	3 (1%)	0	100	100
1	III	217/231 (94%)	213 (98%)	4 (2%)	0	100	100
2	LLL	213/214 (100%)	206 (97%)	7 (3%)	0	100	100
2	MMM	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
All	All	867/890 (97%)	843 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	HHH	199/203 (98%)	196 (98%)	3 (2%)	65 69
1	III	193/203 (95%)	190 (98%)	3 (2%)	62 67
2	LLL	191/190 (100%)	191 (100%)	0	100 100
2	MMM	190/190 (100%)	184 (97%)	6 (3%)	39 38
All	All	773/786 (98%)	761 (98%)	12 (2%)	62 67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	156	PRO
1	HHH	158	PRO
1	HHH	187	LEU
1	III	156	PRO
1	III	158	PRO
1	III	206	ASN
2	MMM	10	SER
2	MMM	20	THR
2	MMM	24	SER
2	MMM	83	ILE
2	MMM	106	ILE
2	MMM	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (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, 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	HHH	227/231 (98%)	0.04	4 (1%) 68 66	24, 34, 61, 98	0
1	III	221/231 (95%)	0.25	11 (4%) 28 28	28, 44, 77, 92	0
2	LLL	214/214 (100%)	0.04	0 100 100	25, 37, 57, 72	0
2	MMM	214/214 (100%)	0.33	7 (3%) 46 45	33, 60, 80, 92	0
All	All	876/890 (98%)	0.16	22 (2%) 57 56	24, 43, 76, 98	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	III	140	THR	3.8
1	III	1	GLU	3.2
2	MMM	212	GLY	3.2
1	III	200	THR	3.1
2	MMM	203	SER	3.1
1	III	197	ASN	3.0
1	HHH	227	GLU	2.5
2	MMM	201	LEU	2.4
2	MMM	154	LEU	2.4
2	MMM	191	VAL	2.4
1	III	100	GLU	2.4
2	MMM	15	LEU	2.3
1	HHH	197	ASN	2.3
1	HHH	200	THR	2.3
1	III	33	ILE	2.3
1	III	226	VAL	2.2
1	III	3	GLN	2.2
1	III	26	GLY	2.2
1	III	193	VAL	2.1
1	HHH	140	THR	2.1
1	III	27	TYR	2.1
2	MMM	150	VAL	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.