

wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2022 – 03:25 pm GMT

PDB ID : 6TKD

Title : ChiLob 7/4 H2 HC-C228S F(ab')2 Authors : Orr, C.M.; Fisher, H.; Tews, I.

Deposited on : 2019-11-28

Resolution : 1.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) 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)

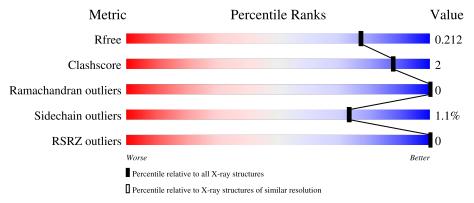
Validation Pipeline (wwPDB-VP) : 2.31.3

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 1.90 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	ННН	231	89%	7% •
2	LLL	214	93%	5% •



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7292 atoms, of which 3379 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 C228S.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	ННН	223	Total 3545	C 1134	H 1739	N 292	O 369	S 11	117	17	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
2	LLL	211	Total 3346	C 1061	H 1640	N 283	O 357	S 5	132	11	0

• Molecule 3 is water.

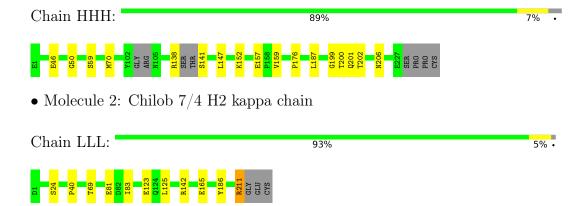
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	ННН	181	Total O 181 181	0	0
3	LLL	220	Total O 220 220	0	0



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: Chilob 7/4 H2 heavy chain C228S





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants	148.02Å 148.02Å 46.14Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	128.19 - 1.90	Depositor
resolution (A)	128.19 - 1.90	EDS
% Data completeness	99.0 (128.19-1.90)	Depositor
(in resolution range)	99.0 (128.19-1.90)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.50 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.173 , 0.206	Depositor
it, it free	0.182 , 0.212	DCC
R_{free} test set	2214 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 56.5	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7292	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	ННН	0.77	0/1848	0.87	0/2515	
2	LLL	0.83	2/1747~(0.1%)	0.91	2/2374 (0.1%)	
All	All	0.80	$2/3595 \ (0.1\%)$	0.89	2/4889 (0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\textup{\AA})$	$\operatorname{Ideal}(\text{\AA})$
2	LLL	81	GLU	CD-OE1	6.34	1.32	1.25
2	LLL	123	GLU	CD-OE2	-5.16	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	<i>y</i> 1		$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	LLL	142	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	LLL	211	ARG	NE-CZ-NH1	-5.19	117.70	120.30

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	ННН	1806	1739	1717	10	0
2	LLL	1706	1640	1628	4	0
3	ННН	181	0	0	3	0
3	LLL	220	0	0	0	0
All	All	3913	3379	3345	14	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 2.

The worst 5 of 14 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:HHH:46[B]:GLU:OE1	3:ННН:301:НОН:О	2.15	0.64
1:HHH:138:ARG:O	1:HHH:141:SER:N	2.34	0.61
1:HHH:201[A]:GLN:HG3	1:HHH:202[A]:THR:O	2.00	0.61
2:LLL:186:TYR:CE2	2:LLL:211:ARG:HD3	2.40	0.56
1:HHH:50:GLY:O	1:HHH:70[A]:MET:HE3	2.06	0.56

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	Perce	ntiles	
1	ННН	234/231 (101%)	228 (97%)	6 (3%)	0	100	100
2	LLL	$220/214\ (103\%)$	217 (99%)	3 (1%)	0	100	100
All	All	454/445 (102%)	445 (98%)	9 (2%)	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	ННН	205/203~(101%)	202 (98%)	3 (2%)		65	62
2	LLL	198/190 (104%)	197 (100%)	1 (0%)		88	89
All	All	403/393~(102%)	399 (99%)	4 (1%)		73	76

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	ННН	59	SER
1	ННН	176	PRO
1	ННН	206	ASN
2	LLL	83	ILE

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 (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, 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		ZZ>2	$OWAB(A^2)$	Q<0.9
1	ННН	223/231 (96%)	-0.14	0	100	100	18, 31, 56, 86	0
2	LLL	211/214 (98%)	-0.32	0	100	100	17, 23, 36, 46	0
All	All	434/445 (97%)	-0.23	0	100	100	17, 27, 49, 86	0

There are no RSRZ outliers to report.

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.

