Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2022 – 10:17 am BST

PDB ID	:	5DRW
Title	:	Crystal structure of the BCR Fab fragment from subset #4 case CLL183
Authors	:	Minici, C.; Degano, M.
Deposited on	:	2015-09-16
Resolution	:	2.27 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:

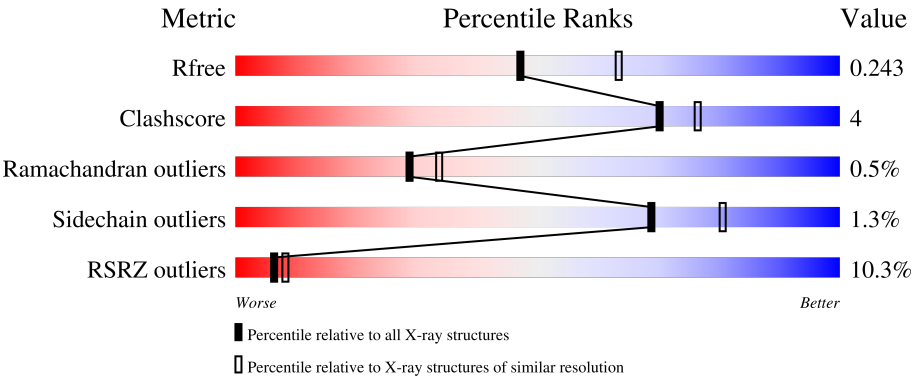
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	226	10% 89% 8% .
2	B	218	10% 87% 12% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3442 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 CLL183 BCR antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1661	1058	275	323	5			

- Molecule 2 is a protein called CLL183 BCR antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1691	1056	292	337	6			

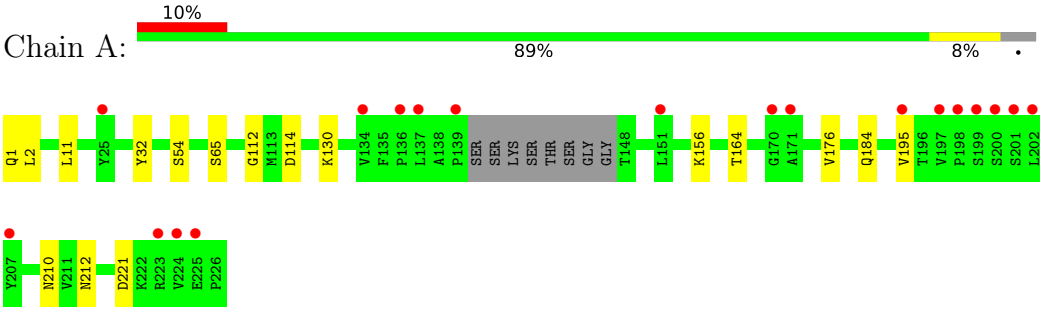
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	32	Total	O	0	0
			32	32		

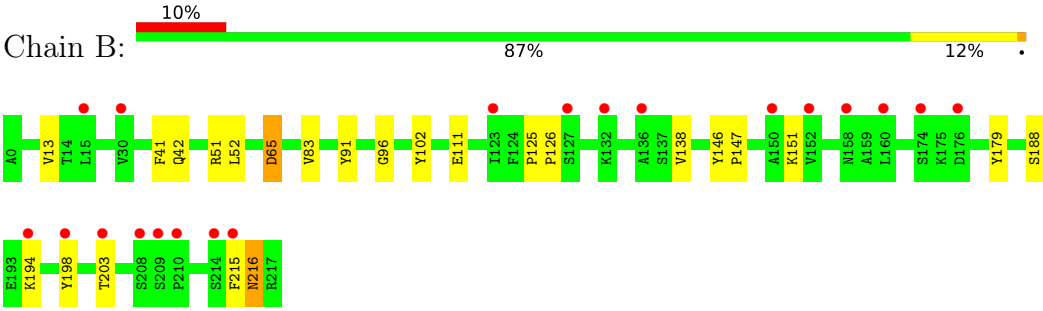
3 Residue-property plots (i)

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: CLL183 BCR antibody heavy chain



• Molecule 2: CLL183 BCR antibody light chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	90.21Å 90.21Å 131.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.66 – 2.27 42.66 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.66-2.27) 99.9 (42.66-2.27)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.27Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.195 , 0.241 0.198 , 0.243	Depositor DCC
R_{free} test set	1319 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3442	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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	0.40	0/1706	0.54	0/2333
2	B	0.36	0/1730	0.53	0/2350
All	All	0.38	0/3436	0.53	0/4683

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	1661	0	1621	8	0
2	B	1691	0	1641	17	0
3	A	58	0	0	1	0
3	B	32	0	0	0	0
All	All	3442	0	3262	24	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 4.

All (24) 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:A:156:LYS:NZ	1:A:184:GLN:OE1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:NZ	3:A:301:HOH:O	2.32	0.63
2:B:111:GLU:OE2	2:B:179:TYR:OH	2.17	0.59
2:B:65:ASP:N	2:B:65:ASP:OD1	2.33	0.59
2:B:188:SER:O	2:B:190:ALA:N	2.33	0.58
2:B:126:PRO:HD3	2:B:138:VAL:HG22	1.85	0.57
2:B:191:ASP:HA	2:B:194:LYS:HE2	1.89	0.54
1:A:176:VAL:HG22	1:A:195:VAL:HG22	1.92	0.52
1:A:1:GLN:HG2	1:A:2:LEU:N	2.26	0.51
2:B:96:GLY:HA2	2:B:102:TYR:CD1	2.48	0.49
2:B:192:TYR:O	2:B:198:TYR:OH	2.30	0.49
2:B:146:TYR:CG	2:B:147:PRO:HA	2.50	0.46
2:B:96:GLY:HA2	2:B:102:TYR:HD1	1.81	0.45
1:A:114:ASP:HB3	2:B:51:ARG:CZ	2.48	0.44
2:B:151:LYS:HD3	2:B:203:THR:HB	1.99	0.44
2:B:125:PRO:HB3	2:B:215:PHE:CE1	2.53	0.44
2:B:13:VAL:HG11	2:B:83:VAL:HG21	2.00	0.44
2:B:126:PRO:HG2	2:B:192:TYR:CE1	2.52	0.43
2:B:41:PHE:O	2:B:91:TYR:HA	2.17	0.43
1:A:210:ASN:ND2	1:A:221:ASP:OD1	2.35	0.42
1:A:164:THR:OG1	1:A:212:ASN:HB2	2.20	0.42
2:B:42:GLN:HB2	2:B:52:LEU:HD11	2.02	0.41
1:A:11:LEU:HD23	1:A:11:LEU:HA	1.92	0.41
2:B:216:ASN:O	2:B:216:ASN:ND2	2.51	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	A	214/226 (95%)	211 (99%)	2 (1%)	1 (0%)	29	34
2	B	216/218 (99%)	210 (97%)	5 (2%)	1 (0%)	29	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	430/444 (97%)	421 (98%)	7 (2%)	2 (0%)	29 34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	189	LYS
1	A	112	GLY

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	186/192 (97%)	183 (98%)	3 (2%)	62 76
2	B	194/194 (100%)	192 (99%)	2 (1%)	76 86
All	All	380/386 (98%)	375 (99%)	5 (1%)	69 80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	54	SER
1	A	65	SER
2	B	65	ASP
2	B	216	ASN

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	A	218/226 (96%)	0.72	23 (10%)	6	8	30, 46, 97, 122	0
2	B	218/218 (100%)	0.70	22 (10%)	7	9	34, 61, 110, 130	0
All	All	436/444 (98%)	0.71	45 (10%)	6	8	30, 53, 107, 130	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	THR	7.0
1	A	207	TYR	6.5
1	A	202	LEU	6.3
2	B	136	ALA	5.3
1	A	223	ARG	5.0
2	B	209	SER	4.6
2	B	158	ASN	4.6
1	A	205	GLN	4.5
1	A	139	PRO	4.0
2	B	150	ALA	4.0
1	A	200	SER	4.0
1	A	203	GLY	3.9
1	A	201	SER	3.9
2	B	215	PHE	3.8
1	A	206	THR	3.8
1	A	151	LEU	3.8
2	B	190	ALA	3.5
2	B	208	SER	3.5
1	A	134	VAL	3.4
2	B	152	VAL	3.3
1	A	199	SER	3.3
2	B	160	LEU	3.2
2	B	214	SER	3.2
1	A	197	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	132	LYS	3.1
1	A	198	PRO	3.0
2	B	123	ILE	3.0
2	B	15	LEU	3.0
1	A	225	GLU	2.9
1	A	25	TYR	2.8
2	B	203	THR	2.8
2	B	127	SER	2.7
2	B	198	TYR	2.7
1	A	195	VAL	2.6
2	B	210	PRO	2.5
1	A	171	ALA	2.5
1	A	224	VAL	2.4
2	B	30	VAL	2.4
1	A	137	LEU	2.3
1	A	136	PRO	2.3
2	B	189	LYS	2.2
2	B	174	SER	2.1
1	A	170	GLY	2.0
2	B	176	ASP	2.0
2	B	194	LYS	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.