

wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 08:46 PM JST

PDB ID : 7DHA

Title: crystal structure of CD38 in complex with daratumumab

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Deposited on : 2020-11-13

Resolution : 2.55 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: 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

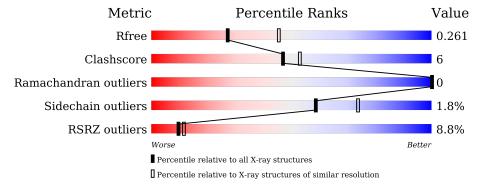
 $Validation\ Pipeline\ (wwPDB-VP) \quad : \quad 2.36$

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 2.55 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	1284 (2.56-2.52)		
Clashscore	141614	1332 (2.56-2.52)		
Ramachandran outliers	138981	1315 (2.56-2.52)		
Sidechain outliers	138945	1315 (2.56-2.52)		
RSRZ outliers	127900	1272 (2.56-2.52)		

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 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	265	74%	20%	6%
2	В	214	7%86%	1	3% •
3	С	234	7% 83%	11%	• 5%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5425 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 ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	248	Total	С	N	О	S	0	0	0
1	A	240	2001	1263	342	380	16	0	U	U

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ASP	ASN	engineered mutation	UNP P28907
A	120	ALA	ASN	engineered mutation	UNP P28907
A	165	ASP	ASN	engineered mutation	UNP P28907
A	175	ASP	ASN	engineered mutation	UNP P28907
A	257	GLY	-	expression tag	UNP P28907
A	258	THR	-	expression tag	UNP P28907
A	259	LYS	-	expression tag	UNP P28907
A	260	HIS	-	expression tag	UNP P28907
A	261	HIS	-	expression tag	UNP P28907
A	262	HIS	-	expression tag	UNP P28907
A	263	HIS	-	expression tag	UNP P28907
A	264	HIS	-	expression tag	UNP P28907
A	265	HIS	-	expression tag	UNP P28907

• Molecule 2 is a protein called Light chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	212	Total 1631	C 1021	N 278	O 328	S 4	0	0	0

• Molecule 3 is a protein called Heavy Chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	222	Total 1650	C 1048	N 273	O 323	S 6	0	0	0



• Molecule 4 is water.

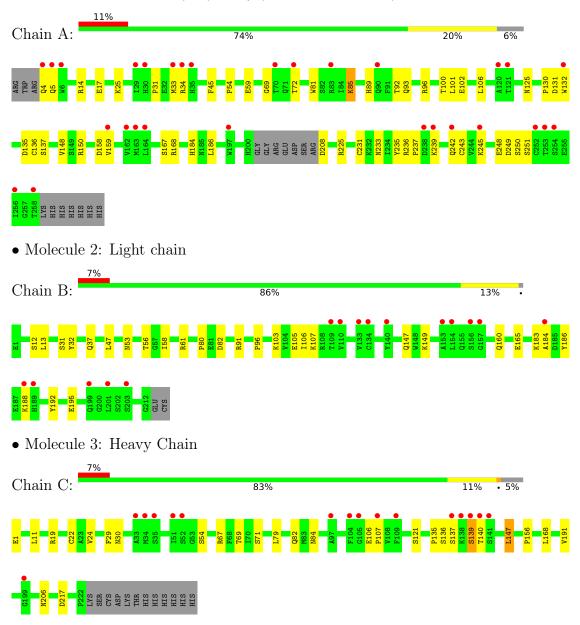
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	55	Total O 55 55	0	0
4	В	34	Total O 34 34	0	0
4	С	54	Total O 54 54	0	0



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: ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants	80.24Å 54.16Å 92.69Å	Donositor
a, b, c, α , β , γ	90.00° 98.88° 90.00°	Depositor
Resolution (Å)	29.09 - 2.55	Depositor
rtesolution (A)	29.09 - 2.55	EDS
% Data completeness	98.0 (29.09-2.55)	Depositor
(in resolution range)	98.0 (29.09-2.55)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.74 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
D D.	0.207 , 0.261	Depositor
R, R_{free}	0.207 , 0.261	DCC
R_{free} test set	2000 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 40.8	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	0.93	EDS
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.27% 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	Bond	lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.30	0/2049	0.48	1/2777 (0.0%)	
2	В	0.28	0/1668	0.49	0/2269	
3	С	0.29	0/1691	0.51	0/2302	
All	All	0.29	0/5408	0.49	1/7348 (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
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	34	ARG	NE-CZ-NH1	6.43	123.52	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	PRO	Peptide

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	A	2001	0	1935	32	0
2	В	1631	0	1587	20	0
3	С	1650	0	1618	16	0
4	A	55	0	0	3	1
4	В	34	0	0	6	1
4	С	54	0	0	3	0
All	All	5425	0	5140	65	1

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 65 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:A:69:GLY:HA3	1:A:106:LEU:HD11	1.49	0.94
2:B:160:GLN:NE2	4:B:302:HOH:O	2.04	0.89
2:B:53:ASN:OD1	4:B:301:HOH:O	2.00	0.78
1:A:242:GLN:HA	1:A:245:LYS:HD2	1.67	0.75
1:A:33:MET:HG3	1:A:72:THR:H	1.50	0.74

All (1) 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-1 Atom-2		Clash overlap (Å)	
4:A:329:HOH:O	4:B:329:HOH:O[2_656]	2.15	0.05	

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	entiles
1	A	244/265 (92%)	231 (95%)	13 (5%)	0	100	100
2	В	210/214 (98%)	202 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$_{ m ntiles}$
3	С	220/234 (94%)	214 (97%)	6 (3%)	0	100	100
All	All	674/713 (94%)	647 (96%)	27 (4%)	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	A	229/244~(94%)	223 (97%)	6 (3%)	46 61
2	В	184/186 (99%)	183 (100%)	1 (0%)	88 93
3	С	184/196 (94%)	180 (98%)	4 (2%)	52 66
All	All	597/626 (95%)	586 (98%)	11 (2%)	59 74

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	С	19	ARG
3	С	30	ASN
3	С	147	LEU
3	С	139	SER
1	A	168	ARG

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

Mol	Chain	Res	Type
1	A	242	GLN
1	A	246	ASN
2	В	166	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 (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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	248/265~(93%)	0.66	29 (11%) 4 6	32, 50, 79, 107	0
2	В	212/214 (99%)	0.43	15 (7%) 16 19	30, 54, 80, 94	0
3	С	222/234 (94%)	0.28	16 (7%) 15 18	28, 39, 61, 124	0
All	All	682/713 (95%)	0.47	60 (8%) 10 11	28, 47, 79, 124	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	С	139	SER	7.7
1	A	34	ARG	6.8
3	С	138	LYS	6.4
3	С	140	THR	5.5
2	В	201	LEU	4.5

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.

