



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2022 – 03:11 pm GMT

PDB ID : 7PHV
Title : PfCyRPA bound to monoclonal antibody Cy.007 Fab fragment
Authors : Ragotte, R.J.; Higgins, M.K.
Deposited on : 2021-08-18
Resolution : 3.09 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 ⓘ symbol.

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 : 2.26
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) : 2.26

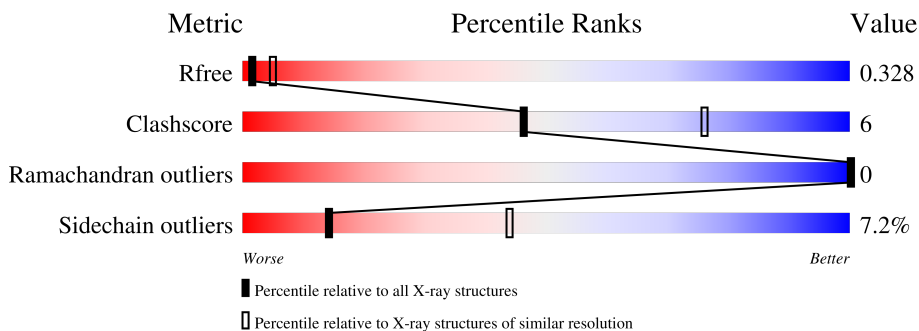
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	343	69% (green), 21% (yellow), 8% (orange), 2% (red), 2% (grey)
1	D	343	69% (green), 19% (yellow), 11% (orange), 1% (red), 2% (grey)
2	B	233	82% (green), 12% (yellow), 5% (orange), 1% (red), 2% (grey)
2	E	233	81% (green), 12% (yellow), 6% (orange), 1% (red), 2% (grey)
3	C	209	91% (green), 7% (yellow), 2% (orange), 1% (red), 2% (grey)
3	F	209	90% (green), 8% (yellow), 2% (orange), 1% (red), 2% (grey)

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11521 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 Cysteine-rich protective antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2633	1697	420	503	13	0	0	0
1	D	305	2539	1640	404	483	12	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	SER	conflict	UNP Q8IFM8
A	324	ALA	THR	conflict	UNP Q8IFM8
A	340	ALA	THR	conflict	UNP Q8IFM8
A	363	GLY	-	expression tag	UNP Q8IFM8
A	364	GLY	-	expression tag	UNP Q8IFM8
A	365	GLY	-	expression tag	UNP Q8IFM8
A	366	GLY	-	expression tag	UNP Q8IFM8
A	367	SER	-	expression tag	UNP Q8IFM8
A	368	GLU	-	expression tag	UNP Q8IFM8
A	369	PRO	-	expression tag	UNP Q8IFM8
A	370	GLU	-	expression tag	UNP Q8IFM8
A	371	ALA	-	expression tag	UNP Q8IFM8
D	147	ALA	SER	conflict	UNP Q8IFM8
D	324	ALA	THR	conflict	UNP Q8IFM8
D	340	ALA	THR	conflict	UNP Q8IFM8
D	363	GLY	-	expression tag	UNP Q8IFM8
D	364	GLY	-	expression tag	UNP Q8IFM8
D	365	GLY	-	expression tag	UNP Q8IFM8
D	366	GLY	-	expression tag	UNP Q8IFM8
D	367	SER	-	expression tag	UNP Q8IFM8
D	368	GLU	-	expression tag	UNP Q8IFM8
D	369	PRO	-	expression tag	UNP Q8IFM8
D	370	GLU	-	expression tag	UNP Q8IFM8
D	371	ALA	-	expression tag	UNP Q8IFM8

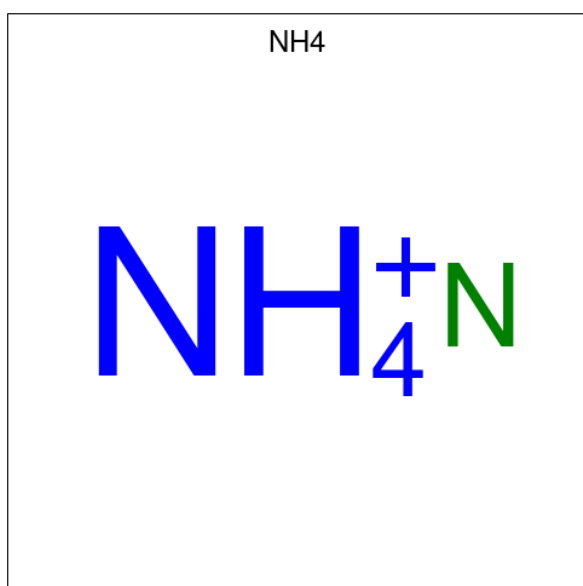
- Molecule 2 is a protein called Monoclonal antibody Cy.007 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	221	Total	C	N	O	S	518	0	0
			1619	1013	272	327	7			
2	E	220	Total	C	N	O	S	646	0	0
			1614	1010	271	326	7			

- Molecule 3 is a protein called Monoclonal antibody Cy.007 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	Total	C	N	O	S	549	0	0
			1557	965	265	323	4			
3	F	207	Total	C	N	O	S	489	0	0
			1557	965	265	323	4			

- Molecule 4 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).

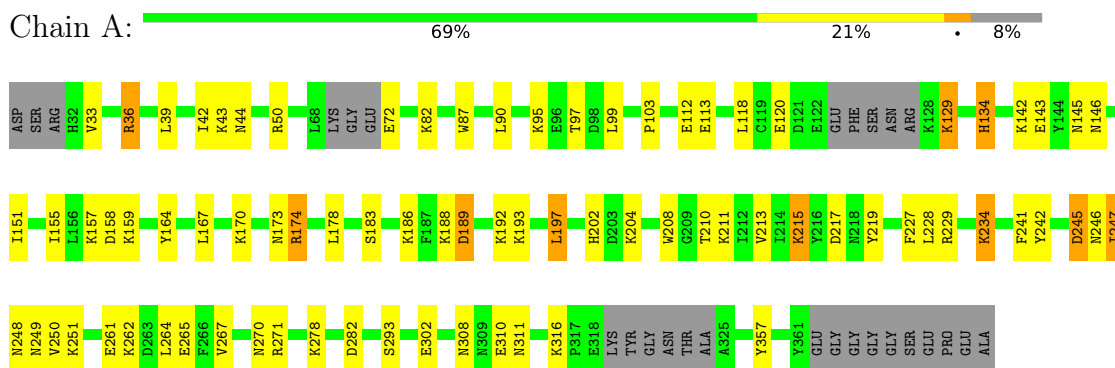


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	N		
4	B	1	Total	N	0	0
			1	1		
4	E	1	Total	N	0	0
			1	1		

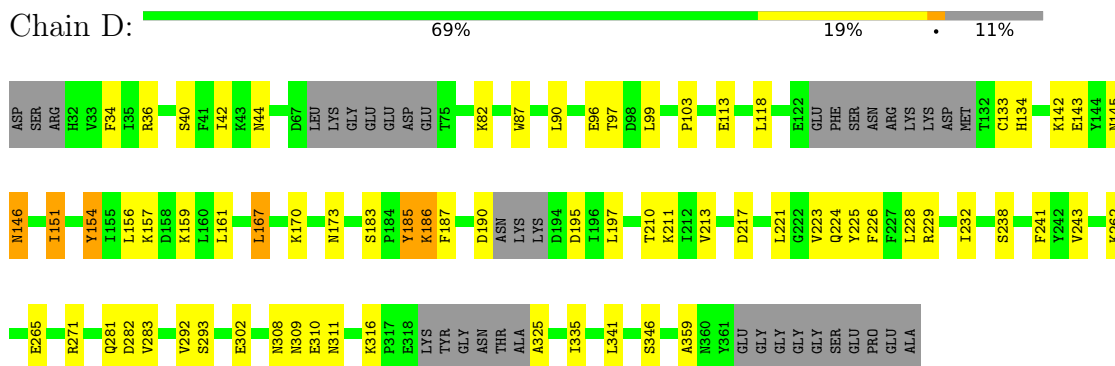
3 Residue-property plots [i](#)

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. 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. 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.

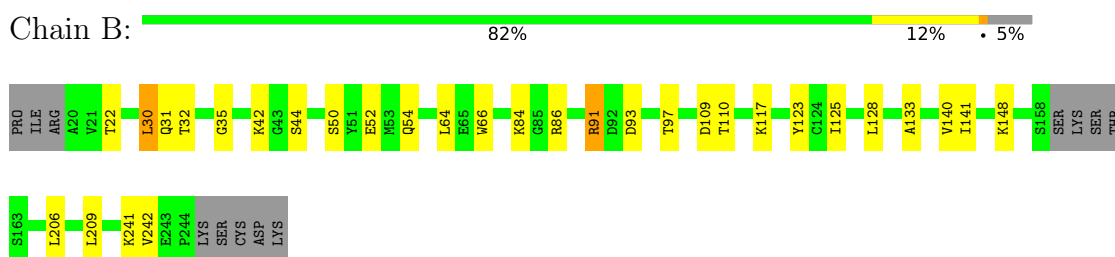
- Molecule 1: Cysteine-rich protective antigen




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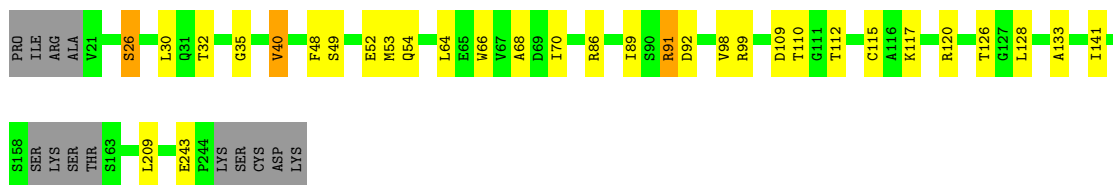


- Molecule 2: Monoclonal antibody Cy.007 heavy chain



- Molecule 2: Monoclonal antibody Cy.007 heavy chain

Chain E:  81% 12% 6%




- Molecule 3: Monoclonal antibody Cy.007 light chain

Chain C:  91% 7%



- Molecule 3: Monoclonal antibody Cy.007 light chain

Chain F:  90% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.10Å 87.00Å 342.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.24 – 3.09 45.24 – 3.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.24-3.09) 99.9 (45.24-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.06Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.287 , 0.332 0.290 , 0.328	Depositor DCC
R_{free} test set	2060 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	109.4	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	11521	wwPDB-VP
Average B, all atoms (Å ²)	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH4

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	0.52	0/2692	0.69	0/3634
1	D	0.46	0/2597	0.64	0/3509
2	B	0.31	0/1654	0.47	0/2254
2	E	0.29	0/1649	0.46	0/2247
3	C	0.26	0/1590	0.42	0/2163
3	F	0.26	0/1590	0.42	0/2163
All	All	0.39	0/11772	0.56	0/15970

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 [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	2633	0	2528	40	0
1	D	2539	0	2429	37	0
2	B	1619	0	1570	12	0
2	E	1614	0	1565	16	0
3	C	1557	0	1493	5	0
3	F	1557	0	1493	7	0
4	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	1	0
All	All	11521	0	11078	114	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 6.

The worst 5 of 114 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:D:325:ALA:HB1	1:D:346:SER:HB2	1.63	0.81
1:A:134:HIS:CE1	1:A:146:ASN:HD22	2.02	0.77
2:B:52:GLU:OE1	4:B:301:NH4:N	2.19	0.75
3:F:108:ARG:HA	3:F:113:GLY:HA2	1.71	0.73
2:E:92:ASP:HB2	2:E:99:ARG:HH12	1.53	0.72

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	308/343 (90%)	289 (94%)	19 (6%)	0	100	100
1	D	295/343 (86%)	270 (92%)	25 (8%)	0	100	100
2	B	217/233 (93%)	207 (95%)	10 (5%)	0	100	100
2	E	216/233 (93%)	204 (94%)	12 (6%)	0	100	100
3	C	205/209 (98%)	193 (94%)	12 (6%)	0	100	100
3	F	205/209 (98%)	189 (92%)	16 (8%)	0	100	100
All	All	1446/1570 (92%)	1352 (94%)	94 (6%)	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	297/316 (94%)	264 (89%)	33 (11%)	6	24
1	D	286/316 (90%)	265 (93%)	21 (7%)	14	43
2	B	179/191 (94%)	168 (94%)	11 (6%)	18	49
2	E	179/191 (94%)	169 (94%)	10 (6%)	21	52
3	C	177/179 (99%)	168 (95%)	9 (5%)	24	56
3	F	177/179 (99%)	168 (95%)	9 (5%)	24	56
All	All	1295/1372 (94%)	1202 (93%)	93 (7%)	14	44

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	146	ASN
1	D	271	ARG
1	D	154	TYR
1	D	210	THR
2	E	30	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	145	ASN
1	A	311	ASN
1	D	145	ASN

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](#)

Of 2 ligands modelled in this entry, 2 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.