



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 24, 2025 – 06:04 AM EST

PDB ID : 9EHT / pdb_00009eht
Title : Crystal Structure of PD-1/retifanimab complex
Authors : Heo, Y.-S.
Deposited on : 2024-11-25
Resolution : 1.54 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 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

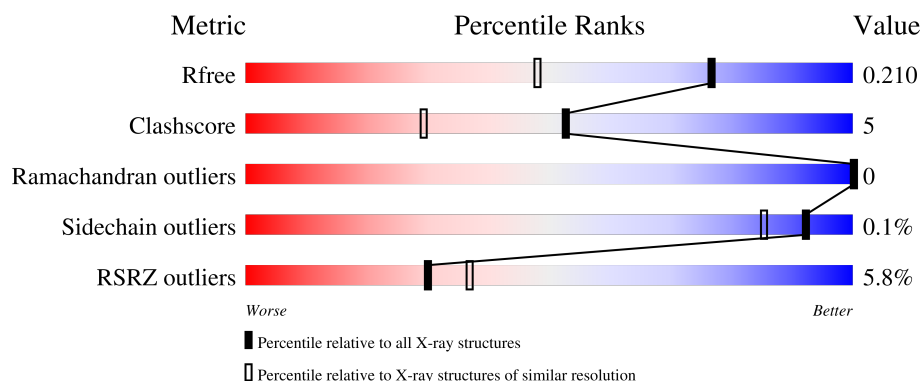
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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}	164625	3511 (1.56-1.52)
Clashscore	180529	3784 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)
RSRZ outliers	164620	3510 (1.56-1.52)

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 $\leq 5\%$. 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	218	<div> <div></div> <div>86% 11% ..</div> </div>
1	D	218	<div> <div></div> <div>88% 10% ..</div> </div>
2	B	231	<div> <div>6%</div> <div>88% 7% .</div> </div>
2	E	231	<div> <div>6%</div> <div>86% 8% . .</div> </div>
3	F	125	<div> <div>13%</div> <div>77% 12% 11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	J	125	<div><div></div><div></div><div></div><div></div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9868 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1648	1032	276	334	6			
1	D	216	Total	C	N	O	S	0	0	0
			1648	1032	276	334	6			

- Molecule 2 is a protein called heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1669	1057	276	330	6			
2	E	221	Total	C	N	O	S	0	0	0
			1669	1057	276	330	6			

- Molecule 3 is a protein called Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	111	Total	C	N	O	S	0	0	0
			885	551	163	167	4			
3	J	110	Total	C	N	O	S	0	0	0
			861	535	157	165	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	93	SER	CYS	conflict	UNP Q15116
J	93	SER	CYS	conflict	UNP Q15116

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	344	Total	O	0	0
			344	344		

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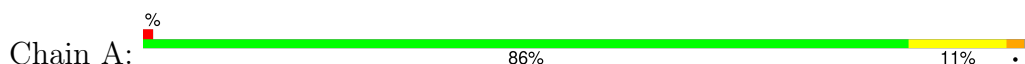
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	351	Total 351	O 351	0	0
4	D	284	Total 284	O 284	0	0
4	E	287	Total 287	O 287	0	0
4	F	94	Total 94	O 94	0	0
4	J	128	Total 128	O 128	0	0

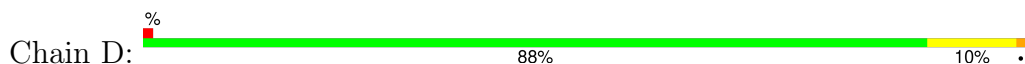
3 Residue-property plots [i](#)

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.

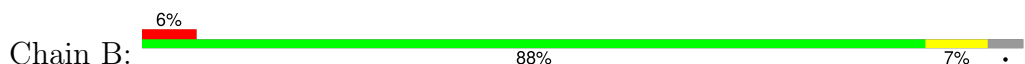
- Molecule 1: light chain



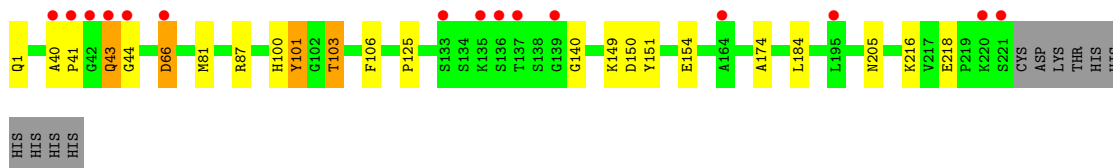
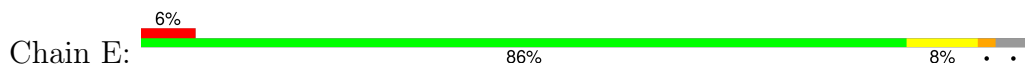
- Molecule 1: light chain



- Molecule 2: heavy chain



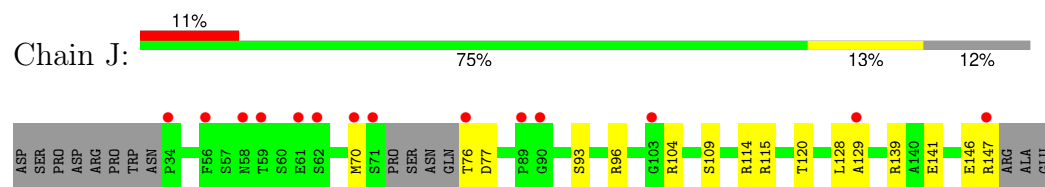
- Molecule 2: heavy chain



- Molecule 3: Programmed cell death protein 1



● Molecule 3: Programmed cell death protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.50Å 93.16Å 89.91Å 90.00° 112.39° 90.00°	Depositor
Resolution (Å)	29.29 – 1.54 29.29 – 1.54	Depositor EDS
% Data completeness (in resolution range)	96.6 (29.29-1.54) 96.6 (29.29-1.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.54Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.181 , 0.208 0.182 , 0.210	Depositor DCC
R_{free} test set	8790 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9868	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% 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

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	0.48	1/1685 (0.1%)	1.11	15/2286 (0.7%)
1	D	0.42	0/1685	1.02	17/2286 (0.7%)
2	B	0.44	0/1713	0.88	4/2337 (0.2%)
2	E	0.42	0/1713	0.87	8/2337 (0.3%)
3	F	0.36	0/903	0.80	5/1221 (0.4%)
3	J	0.33	0/878	0.78	3/1187 (0.3%)
All	All	0.42	1/8577 (0.0%)	0.94	52/11654 (0.4%)

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	5
1	D	0	5
2	B	0	1
2	E	0	1
3	F	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	ALA	N-CA	-5.55	1.38	1.46

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ALA	CA-C-N	16.22	148.51	123.05
1	A	54	ALA	C-N-CA	16.22	148.51	123.05
1	D	54	ALA	CA-C-N	12.90	143.30	123.05
1	D	54	ALA	C-N-CA	12.90	143.30	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	55	ALA	CA-C-N	10.15	137.99	122.37

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ASN	Mainchain
1	A	29	VAL	Mainchain
1	A	36	PHE	Mainchain
1	A	55	ALA	Peptide,Mainchain
2	B	106	PHE	Mainchain

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	1648	0	1595	17	0
1	D	1648	0	1596	13	0
2	B	1669	0	1634	12	0
2	E	1669	0	1634	17	0
3	F	885	0	859	10	0
3	J	861	0	837	14	0
4	A	344	0	0	5	0
4	B	351	0	0	8	6
4	D	284	0	0	4	1
4	E	287	0	0	7	4
4	F	94	0	0	7	1
4	J	128	0	0	7	2
All	All	9868	0	8155	81	7

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 5.

The worst 5 of 81 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)
2:E:40:ALA:HB3	2:E:43:GLN:HG3	1.30	1.05
1:D:37:MET:HB3	1:D:55:ALA:HB2	1.42	1.00
3:J:141:GLU:OE1	4:J:201:HOH:O	1.81	0.97
1:D:43:LYS:NZ	4:D:302:HOH:O	1.96	0.96
1:D:191:GLU:OE1	4:D:301:HOH:O	1.84	0.95

The worst 5 of 7 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-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:569:HOH:O	4:D:534:HOH:O[2_556]	1.82	0.38
4:B:525:HOH:O	4:E:437:HOH:O[2_555]	1.95	0.25
4:E:522:HOH:O	4:J:274:HOH:O[1_554]	2.05	0.15
4:B:316:HOH:O	4:E:425:HOH:O[2_555]	2.06	0.14
4:B:628:HOH:O	4:J:325:HOH:O[2_657]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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	214/218 (98%)	214 (100%)	0	0	100	100
1	D	214/218 (98%)	214 (100%)	0	0	100	100
2	B	219/231 (95%)	219 (100%)	0	0	100	100
2	E	219/231 (95%)	219 (100%)	0	0	100	100
3	F	105/125 (84%)	105 (100%)	0	0	100	100
3	J	106/125 (85%)	106 (100%)	0	0	100	100
All	All	1077/1148 (94%)	1077 (100%)	0	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	188/190 (99%)	188 (100%)	0	100	100
1	D	188/190 (99%)	188 (100%)	0	100	100
2	B	190/200 (95%)	190 (100%)	0	100	100
2	E	190/200 (95%)	189 (100%)	1 (0%)	86	76
3	F	98/110 (89%)	98 (100%)	0	100	100
3	J	95/110 (86%)	95 (100%)	0	100	100
All	All	949/1000 (95%)	948 (100%)	1 (0%)	92	85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	1	GLN

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

Mol	Chain	Res	Type
2	B	205	ASN
1	D	164	GLN
3	F	58	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 oligosaccharides 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, 95th 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	216/218 (99%)	-0.08	3 (1%) 73 80	13, 19, 33, 46	0
1	D	216/218 (99%)	0.21	2 (0%) 81 86	14, 23, 42, 61	0
2	B	221/231 (95%)	0.23	14 (6%) 27 33	14, 21, 43, 55	0
2	E	221/231 (95%)	0.41	15 (6%) 25 30	14, 25, 46, 64	0
3	F	111/125 (88%)	1.14	16 (14%) 7 8	18, 38, 67, 78	0
3	J	110/125 (88%)	0.83	14 (12%) 9 11	21, 31, 58, 65	0
All	All	1095/1148 (95%)	0.35	64 (5%) 30 37	13, 24, 50, 78	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	55	ALA	6.2
1	A	55	ALA	5.5
3	F	32	TRP	5.0
2	B	41	PRO	4.5
3	F	89	PRO	4.1

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 oligosaccharides 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.