



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:57 AM UTC

PDB ID : 8HN4 / pdb_00008hn4
Title : Complex structure of HLA2402 with recognizing SARS-CoV-2 epitope QYIK-WPWYI
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Deposited on : 2022-12-07
Resolution : 2.85 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

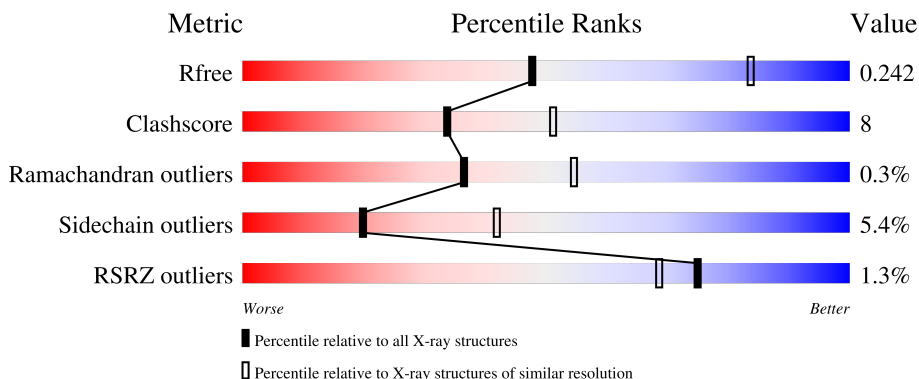
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	308	11% 71% 17% • 11%
2	B	100	85% 15%
3	E	9	11% 33% 44% 11% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3156 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2226	1385	403	428	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP F6IR24
A	21	ASN	-	expression tag	UNP F6IR24
A	22	SER	-	expression tag	UNP F6IR24
A	23	VAL	-	expression tag	UNP F6IR24
A	24	ASP	-	expression tag	UNP F6IR24
A	301	GLY	-	expression tag	UNP F6IR24
A	302	SER	-	expression tag	UNP F6IR24
A	303	GLY	-	expression tag	UNP F6IR24
A	304	LEU	-	expression tag	UNP F6IR24
A	305	ASN	-	expression tag	UNP F6IR24
A	306	ASP	-	expression tag	UNP F6IR24
A	307	ILE	-	expression tag	UNP F6IR24
A	308	PHE	-	expression tag	UNP F6IR24
A	309	GLU	-	expression tag	UNP F6IR24
A	310	ALA	-	expression tag	UNP F6IR24
A	311	GLN	-	expression tag	UNP F6IR24
A	312	LYS	-	expression tag	UNP F6IR24
A	313	ILE	-	expression tag	UNP F6IR24
A	314	GLU	-	expression tag	UNP F6IR24
A	315	TRP	-	expression tag	UNP F6IR24
A	316	HIS	-	expression tag	UNP F6IR24
A	317	ALA	-	expression tag	UNP F6IR24
A	318	ALA	-	expression tag	UNP F6IR24
A	319	ALA	-	expression tag	UNP F6IR24
A	320	LEU	-	expression tag	UNP F6IR24
A	321	GLU	-	expression tag	UNP F6IR24
A	322	HIS	-	expression tag	UNP F6IR24

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Chain	Residue	Modelled	Actual	Comment	Reference
A	323	HIS	-	expression tag	UNP F6IR24
A	324	HIS	-	expression tag	UNP F6IR24
A	325	HIS	-	expression tag	UNP F6IR24
A	326	HIS	-	expression tag	UNP F6IR24
A	327	HIS	-	expression tag	UNP F6IR24

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

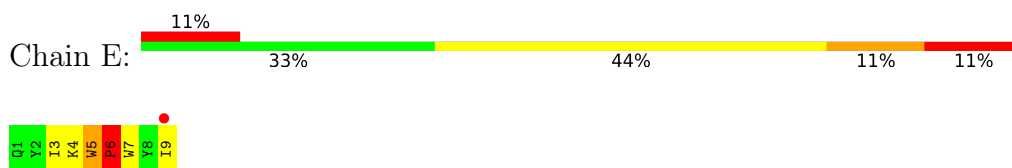
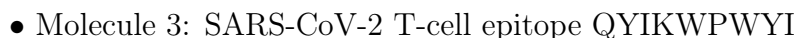
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called SARS-CoV-2 T-cell epitope QYIKWPWYI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			93	68	13	12			

- Molecule 1: MHC class I antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.07Å 67.25Å 116.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.64 – 2.85 39.64 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.64-2.85) 99.5 (39.64-2.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.212 , 0.251 0.205 , 0.242	Depositor DCC
R_{free} test set	458 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3156	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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](#)

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	0.60	2/2286 (0.1%)	0.86	2/3099 (0.1%)
2	B	0.78	2/860 (0.2%)	0.79	0/1162
3	E	1.49	1/99 (1.0%)	1.49	2/136 (1.5%)
All	All	0.69	5/3245 (0.2%)	0.87	4/4397 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASP	C-O	-5.72	1.17	1.24
2	B	38	ASP	C-O	-5.45	1.17	1.23
3	E	6	PRO	C-O	-5.44	1.16	1.24
2	B	50	GLU	C-O	-5.41	1.16	1.23
1	A	30	ARG	C-O	-5.32	1.17	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7	TRP	N-CA-C	6.94	120.37	109.96
3	E	6	PRO	N-CA-CB	-5.85	97.11	103.25
1	A	52	VAL	N-CA-C	-5.42	99.93	107.80
1	A	253	GLU	CB-CA-C	-5.16	101.72	110.19

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	2226	0	2082	36	0
2	B	837	0	803	14	0
3	E	93	0	90	6	0
All	All	3156	0	2975	47	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 8.

All (47) 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:171:TRP:CH2	3:E:5:TRP:HH2	1.77	1.01
1:A:171:TRP:CH2	3:E:5:TRP:CH2	2.69	0.79
1:A:153:ASP:HB2	1:A:155:ARG:HH11	1.50	0.74
2:B:47:GLU:H	2:B:47:GLU:CD	1.99	0.70
1:A:171:TRP:CZ2	3:E:5:TRP:HH2	2.12	0.67
2:B:23:LEU:HD23	2:B:39:LEU:HD22	1.77	0.67
2:B:23:LEU:CD2	2:B:39:LEU:HD22	2.28	0.63
2:B:41:LYS:HG3	2:B:78:TYR:CE1	2.33	0.62
1:A:79:GLU:OE1	1:A:194:ARG:NH1	2.32	0.61
1:A:153:ASP:HB2	1:A:155:ARG:NH1	2.19	0.58
1:A:258:ARG:NH1	2:B:99:MET:SD	2.73	0.58
1:A:171:TRP:CZ2	3:E:5:TRP:CH2	2.90	0.57
2:B:49:VAL:HA	2:B:68:THR:HG23	1.86	0.57
1:A:29:MET:HB2	1:A:192:LEU:HD13	1.85	0.57
1:A:244:ASP:OD2	1:A:280:ARG:NH2	2.32	0.57
1:A:45:ARG:HE	1:A:47:ILE:HD11	1.69	0.56
1:A:226:ARG:NH1	2:B:98:ASP:O	2.36	0.56
2:B:96:ASP:HB3	2:B:99:MET:HA	1.87	0.56
1:A:254:LEU:HD11	1:A:267:LYS:HE3	1.89	0.54
1:A:226:ARG:HD2	2:B:98:ASP:OD1	2.08	0.54
1:A:127:VAL:HG13	1:A:192:LEU:HD23	1.92	0.52
1:A:131:GLY:O	1:A:193:ARG:HD3	2.12	0.49
1:A:226:ARG:HE	1:A:270:ALA:HB2	1.80	0.46
1:A:239:LEU:HD23	1:A:285:VAL:HG22	1.97	0.46
1:A:73:ALA:O	1:A:76:ILE:HG22	2.16	0.46
1:A:262:ASP:OD1	1:A:264:THR:OG1	2.33	0.46
1:A:201:GLU:C	1:A:205:ARG:HD2	2.42	0.45
1:A:44:PRO:HG2	1:A:99:ARG:HG2	1.98	0.45
3:E:5:TRP:CD1	3:E:5:TRP:O	2.70	0.45
1:A:236:GLU:H	1:A:236:GLU:CD	2.25	0.45
1:A:135:ARG:CZ	1:A:152:GLU:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:O	1:A:152:GLU:HG3	2.18	0.44
1:A:94:HIS:NE2	1:A:121:MET:SD	2.92	0.43
1:A:215:HIS:NE2	1:A:278:GLU:OE2	2.51	0.43
1:A:207:ASP:OD1	1:A:207:ASP:N	2.51	0.43
1:A:219:SER:OG	1:A:220:ASP:N	2.51	0.42
2:B:49:VAL:HA	2:B:68:THR:CG2	2.48	0.42
1:A:153:ASP:CG	1:A:155:ARG:HG2	2.44	0.42
2:B:23:LEU:O	2:B:67:TYR:HA	2.20	0.42
1:A:268:TRP:NE1	2:B:99:MET:SD	2.78	0.41
1:A:45:ARG:NE	1:A:47:ILE:HD11	2.35	0.41
1:A:180:GLN:OE1	3:E:3:ILE:HD11	2.21	0.41
1:A:238:THR:HB	1:A:286:GLN:HB2	2.02	0.41
1:A:135:ARG:NE	1:A:152:GLU:OE1	2.53	0.41
1:A:169:ARG:HH11	1:A:169:ARG:HD2	1.75	0.41
2:B:49:VAL:HG22	2:B:68:THR:CG2	2.50	0.41
2:B:49:VAL:HG22	2:B:68:THR:HG23	2.03	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	272/308 (88%)	263 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	E	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	0
All	All	377/417 (90%)	364 (97%)	12 (3%)	1 (0%)	36	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	6	PRO

5.3.2 Protein sidechains ⓘ

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	231/258 (90%)	219 (95%)	12 (5%)	21	43
2	B	95/95 (100%)	93 (98%)	2 (2%)	47	70
3	E	9/9 (100%)	5 (56%)	4 (44%)	0	0
All	All	335/362 (92%)	317 (95%)	18 (5%)	20	42

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	58	VAL
1	A	99	ARG
1	A	134	LEU
1	A	170	LYS
1	A	181	ARG
1	A	189	VAL
1	A	202	THR
1	A	207	ASP
1	A	240	THR
1	A	278	GLU
1	A	292	LYS
2	B	44	GLU
2	B	94	LYS
3	E	4	LYS
3	E	5	TRP
3	E	6	PRO
3	E	9	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	GLN
2	B	42	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	274/308 (88%)	-0.01	3 (1%) 78 73	14, 31, 51, 77	0
2	B	100/100 (100%)	-0.20	1 (1%) 79 74	15, 25, 44, 49	0
3	E	9/9 (100%)	0.35	1 (11%) 10 8	22, 28, 38, 41	0
All	All	383/417 (91%)	-0.05	5 (1%) 75 68	14, 30, 49, 77	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	69	GLU	3.2
1	A	132	ARG	2.3
3	E	9	ILE	2.2
1	A	220	ASP	2.2
1	A	99	ARG	2.1

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.