



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:32 AM UTC

PDB ID : 8ZX7 / pdb_00008zx7
Title : Crystal structure of HCoV-OC43 fusion core
Authors : Lei, Y.
Deposited on : 2024-06-13
Resolution : 3.34 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

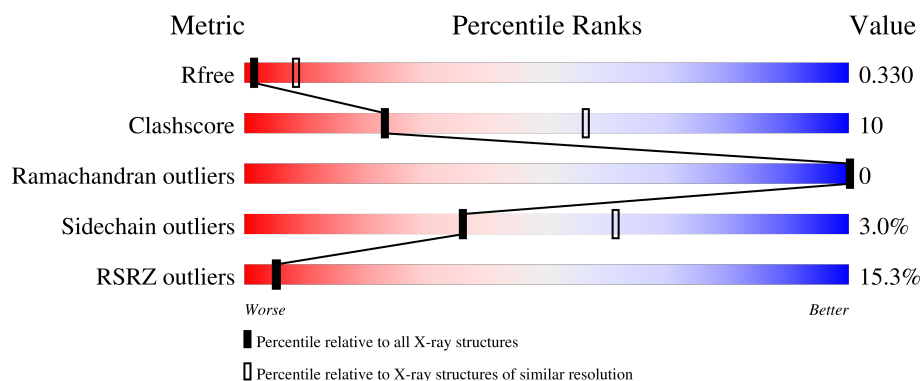
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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	118	7% 45% 13% . 42%
1	B	118	12% 43% 13% . 43%
1	C	118	8% 44% 12% . 43%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1564 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 Spike protein S2'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			532	331	92	108	1			
1	B	67	Total	C	N	O	S	0	0	0
			516	321	89	105	1			
1	C	67	Total	C	N	O	S	0	0	0
			516	321	89	105	1			

There are 153 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASP	TYR	conflict	UNP P36334
A	57A	GLY	-	linker	UNP P36334
A	57B	GLY	-	linker	UNP P36334
A	57C	GLY	-	linker	UNP P36334
A	57D	GLY	-	linker	UNP P36334
A	57E	GLY	-	linker	UNP P36334
A	57F	GLY	-	linker	UNP P36334
A	57G	GLY	-	linker	UNP P36334
A	57H	GLY	-	linker	UNP P36334
A	57I	GLY	-	linker	UNP P36334
A	57J	GLY	-	linker	UNP P36334
A	57K	GLY	-	linker	UNP P36334
A	57L	GLY	-	linker	UNP P36334
A	57M	GLY	-	linker	UNP P36334
A	57N	GLY	-	linker	UNP P36334
A	57O	GLY	-	linker	UNP P36334
A	57P	GLY	-	linker	UNP P36334
A	57Q	GLY	-	linker	UNP P36334
A	57R	GLY	-	linker	UNP P36334
A	57S	GLY	-	linker	UNP P36334
A	57T	GLY	-	linker	UNP P36334
A	57U	GLY	-	linker	UNP P36334
A	57V	GLY	-	linker	UNP P36334

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	57W	GLY	-	linker	UNP P36334
A	57X	GLY	-	linker	UNP P36334
A	57Y	GLY	-	linker	UNP P36334
A	57Z	GLY	-	linker	UNP P36334
A	58A	GLY	-	linker	UNP P36334
A	58B	GLY	-	linker	UNP P36334
A	58C	GLY	-	linker	UNP P36334
A	58D	GLY	-	linker	UNP P36334
A	58E	GLY	-	linker	UNP P36334
A	58F	GLY	-	linker	UNP P36334
A	58G	GLY	-	linker	UNP P36334
A	58H	GLY	-	linker	UNP P36334
A	58I	GLY	-	linker	UNP P36334
A	58J	GLY	-	linker	UNP P36334
A	58K	GLY	-	linker	UNP P36334
A	58L	GLY	-	linker	UNP P36334
A	58M	GLY	-	linker	UNP P36334
A	58N	GLY	-	linker	UNP P36334
A	58O	GLY	-	linker	UNP P36334
A	58P	GLY	-	linker	UNP P36334
A	58Q	GLY	-	linker	UNP P36334
A	58R	GLY	-	linker	UNP P36334
A	58S	GLY	-	linker	UNP P36334
A	58T	GLY	-	linker	UNP P36334
A	58U	GLY	-	linker	UNP P36334
A	58V	GLY	-	linker	UNP P36334
A	58W	GLY	-	linker	UNP P36334
A	101	ASP	VAL	conflict	UNP P36334
B	25	ASP	TYR	conflict	UNP P36334
B	57A	GLY	-	linker	UNP P36334
B	57B	GLY	-	linker	UNP P36334
B	57C	GLY	-	linker	UNP P36334
B	57D	GLY	-	linker	UNP P36334
B	57E	GLY	-	linker	UNP P36334
B	57F	GLY	-	linker	UNP P36334
B	57G	GLY	-	linker	UNP P36334
B	57H	GLY	-	linker	UNP P36334
B	57I	GLY	-	linker	UNP P36334
B	57J	GLY	-	linker	UNP P36334
B	57K	GLY	-	linker	UNP P36334
B	57L	GLY	-	linker	UNP P36334
B	57M	GLY	-	linker	UNP P36334

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	57N	GLY	-	linker	UNP P36334
B	57O	GLY	-	linker	UNP P36334
B	57P	GLY	-	linker	UNP P36334
B	57Q	GLY	-	linker	UNP P36334
B	57R	GLY	-	linker	UNP P36334
B	57S	GLY	-	linker	UNP P36334
B	57T	GLY	-	linker	UNP P36334
B	57U	GLY	-	linker	UNP P36334
B	57V	GLY	-	linker	UNP P36334
B	57W	GLY	-	linker	UNP P36334
B	57X	GLY	-	linker	UNP P36334
B	57Y	GLY	-	linker	UNP P36334
B	57Z	GLY	-	linker	UNP P36334
B	58A	GLY	-	linker	UNP P36334
B	58B	GLY	-	linker	UNP P36334
B	58C	GLY	-	linker	UNP P36334
B	58D	GLY	-	linker	UNP P36334
B	58E	GLY	-	linker	UNP P36334
B	58F	GLY	-	linker	UNP P36334
B	58G	GLY	-	linker	UNP P36334
B	58H	GLY	-	linker	UNP P36334
B	58I	GLY	-	linker	UNP P36334
B	58J	GLY	-	linker	UNP P36334
B	58K	GLY	-	linker	UNP P36334
B	58L	GLY	-	linker	UNP P36334
B	58M	GLY	-	linker	UNP P36334
B	58N	GLY	-	linker	UNP P36334
B	58O	GLY	-	linker	UNP P36334
B	58P	GLY	-	linker	UNP P36334
B	58Q	GLY	-	linker	UNP P36334
B	58R	GLY	-	linker	UNP P36334
B	58S	GLY	-	linker	UNP P36334
B	58T	GLY	-	linker	UNP P36334
B	58U	GLY	-	linker	UNP P36334
B	58V	GLY	-	linker	UNP P36334
B	58W	GLY	-	linker	UNP P36334
B	101	ASP	VAL	conflict	UNP P36334
C	25	ASP	TYR	conflict	UNP P36334
C	57A	GLY	-	linker	UNP P36334
C	57B	GLY	-	linker	UNP P36334
C	57C	GLY	-	linker	UNP P36334
C	57D	GLY	-	linker	UNP P36334

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	57E	GLY	-	linker	UNP P36334
C	57F	GLY	-	linker	UNP P36334
C	57G	GLY	-	linker	UNP P36334
C	57H	GLY	-	linker	UNP P36334
C	57I	GLY	-	linker	UNP P36334
C	57J	GLY	-	linker	UNP P36334
C	57K	GLY	-	linker	UNP P36334
C	57L	GLY	-	linker	UNP P36334
C	57M	GLY	-	linker	UNP P36334
C	57N	GLY	-	linker	UNP P36334
C	57O	GLY	-	linker	UNP P36334
C	57P	GLY	-	linker	UNP P36334
C	57Q	GLY	-	linker	UNP P36334
C	57R	GLY	-	linker	UNP P36334
C	57S	GLY	-	linker	UNP P36334
C	57T	GLY	-	linker	UNP P36334
C	57U	GLY	-	linker	UNP P36334
C	57V	GLY	-	linker	UNP P36334
C	57W	GLY	-	linker	UNP P36334
C	57X	GLY	-	linker	UNP P36334
C	57Y	GLY	-	linker	UNP P36334
C	57Z	GLY	-	linker	UNP P36334
C	58A	GLY	-	linker	UNP P36334
C	58B	GLY	-	linker	UNP P36334
C	58C	GLY	-	linker	UNP P36334
C	58D	GLY	-	linker	UNP P36334
C	58E	GLY	-	linker	UNP P36334
C	58F	GLY	-	linker	UNP P36334
C	58G	GLY	-	linker	UNP P36334
C	58H	GLY	-	linker	UNP P36334
C	58I	GLY	-	linker	UNP P36334
C	58J	GLY	-	linker	UNP P36334
C	58K	GLY	-	linker	UNP P36334
C	58L	GLY	-	linker	UNP P36334
C	58M	GLY	-	linker	UNP P36334
C	58N	GLY	-	linker	UNP P36334
C	58O	GLY	-	linker	UNP P36334
C	58P	GLY	-	linker	UNP P36334
C	58Q	GLY	-	linker	UNP P36334
C	58R	GLY	-	linker	UNP P36334
C	58S	GLY	-	linker	UNP P36334
C	58T	GLY	-	linker	UNP P36334

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	58U	GLY	-	linker	UNP P36334
C	58V	GLY	-	linker	UNP P36334
C	58W	GLY	-	linker	UNP P36334
C	101	ASP	VAL	conflict	UNP P36334

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	39.03Å 48.20Å 103.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.19 – 3.34 48.19 – 3.34	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.19-3.34) 94.1 (48.19-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.30 (at 3.33Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.274 , 0.335 0.273 , 0.330	Depositor DCC
R_{free} test set	134 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.5	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	0.83	EDS
Total number of atoms	1564	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.35% 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	0.17	0/534	0.51	0/724
1	B	0.19	0/518	0.43	0/702
1	C	0.19	0/518	0.44	0/702
All	All	0.19	0/1570	0.46	0/2128

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	532	0	523	15	0
1	B	516	0	506	12	0
1	C	516	0	506	13	0
All	All	1564	0	1535	32	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 10.

All (32) 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:28:GLN:NE2	1:A:114:ASN:OD1	2.10	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD13	1:A:92:ILE:HA	1.69	0.75
1:A:29:GLU:HG3	1:C:105:ARG:HH21	1.54	0.70
1:A:35:ASN:HD21	1:A:107:GLN:HG2	1.62	0.65
1:A:53:ASN:HB2	1:A:94:VAL:HG21	1.82	0.61
1:A:28:GLN:HG2	1:A:110:ILE:HG23	1.83	0.60
1:C:42:GLN:HB2	1:C:99:LEU:HD12	1.84	0.60
1:A:35:ASN:ND2	1:A:107:GLN:OE1	2.35	0.59
1:C:23:ALA:O	1:C:27:ILE:HG12	2.04	0.58
1:C:28:GLN:NE2	1:C:114:ASN:OD1	2.38	0.55
1:C:112:VAL:O	1:C:116:SER:OG	2.20	0.54
1:B:27:ILE:HG21	1:C:27:ILE:CD1	2.40	0.51
1:B:21:ASN:ND2	1:B:118:ILE:O	2.41	0.50
1:B:27:ILE:HG21	1:C:27:ILE:HD11	1.96	0.48
1:C:100:GLN:HA	1:C:103:MET:HE3	1.96	0.47
1:A:56:LEU:HB3	1:A:92:ILE:HG12	1.97	0.47
1:B:53:ASN:HB2	1:B:94:VAL:HG21	1.97	0.46
1:B:104:ASN:O	1:B:108:GLU:HG2	2.16	0.46
1:C:108:GLU:O	1:C:108:GLU:HG3	2.16	0.46
1:A:105:ARG:NH2	1:B:32:ASP:HB3	2.32	0.44
1:B:35:ASN:ND2	1:B:107:GLN:OE1	2.51	0.44
1:A:19:ALA:HB1	1:C:116:SER:HB3	2.00	0.44
1:B:38:LEU:HB3	1:B:99:LEU:HD23	1.99	0.44
1:A:29:GLU:HG3	1:C:105:ARG:NH2	2.29	0.43
1:C:101:ASP:O	1:C:105:ARG:HG3	2.18	0.43
1:B:31:PHE:HD1	1:B:31:PHE:HA	1.73	0.42
1:A:24:LEU:HD12	1:A:117:TYR:CD1	2.55	0.42
1:A:20:PHE:O	1:A:24:LEU:HG	2.21	0.41
1:B:97:LEU:HG	1:B:99:LEU:HD13	2.03	0.41
1:A:41:ILE:HG21	1:B:41:ILE:CD1	2.51	0.41
1:C:99:LEU:O	1:C:103:MET:HG3	2.21	0.41
1:A:105:ARG:HE	1:B:33:ALA:HB2	1.86	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	65/118 (55%)	64 (98%)	1 (2%)	0	100	100
1	B	63/118 (53%)	62 (98%)	1 (2%)	0	100	100
1	C	63/118 (53%)	63 (100%)	0	0	100	100
All	All	191/354 (54%)	189 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	57/57 (100%)	56 (98%)	1 (2%)	51	69
1	B	55/57 (96%)	54 (98%)	1 (2%)	51	69
1	C	55/57 (96%)	52 (94%)	3 (6%)	19	48
All	All	167/171 (98%)	162 (97%)	5 (3%)	36	61

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

Mol	Chain	Res	Type
1	A	29	GLU
1	B	99	LEU
1	C	22	ASN
1	C	36	SER
1	C	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	100	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	107	GLN
1	A	119	ASN
1	B	28	GLN
1	B	35	ASN
1	B	93	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

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, 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	69/118 (58%)	1.13	8 (11%) 9 9	13, 26, 36, 51	0
1	B	67/118 (56%)	1.39	14 (20%) 2 3	17, 29, 46, 53	0
1	C	67/118 (56%)	1.07	9 (13%) 7 7	16, 27, 47, 57	0
All	All	203/354 (57%)	1.20	31 (15%) 5 5	13, 27, 47, 57	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	ASP	4.7
1	B	114	ASN	4.1
1	C	108	GLU	3.8
1	B	23	ALA	3.6
1	A	47	ALA	3.6
1	B	26	ALA	3.5
1	B	27	ILE	3.5
1	A	55	LEU	3.1
1	A	27	ILE	3.1
1	C	93	ASN	3.0
1	A	31	PHE	3.0
1	A	50	GLU	3.0
1	C	55	LEU	2.9
1	C	102	GLU	2.9
1	B	36	SER	2.8
1	B	30	GLY	2.7
1	B	17	ALA	2.7
1	C	95	THR	2.6
1	B	51	ALA	2.6
1	C	53	ASN	2.6
1	B	54	ASN	2.5
1	A	36	SER	2.4
1	B	98	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	102	GLU	2.4
1	B	101	ASP	2.3
1	C	117	TYR	2.3
1	A	119	ASN	2.3
1	B	19	ALA	2.2
1	B	107	GLN	2.2
1	C	57	GLN	2.0
1	C	27	ILE	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 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.