



# wwPDB X-ray Structure Validation Summary Report

Mar 9, 2026 – 08:40 AM UTC

PDB ID : 7ZFA / pdb\_00007zfa  
Title : SARS-CoV-2 Omicron RBD in complex with Omi-6 and COVOX-150 Fabs  
Authors : Zhou, D.; Huo, J.; Ren, J.; Stuart, D.I.  
Deposited on : 2022-04-01  
Resolution : 4.24 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](mailto: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>.

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The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

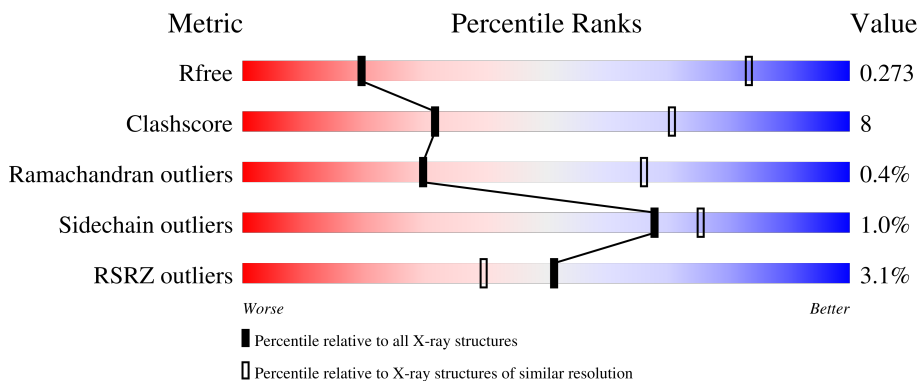
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.24 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	1042 (4.60-3.88)
Clashscore	190562	1043 (4.58-3.90)
Ramachandran outliers	187476	1031 (4.62-3.86)
Sidechain outliers	187428	1016 (4.62-3.86)
RSRZ outliers	180081	1039 (4.60-3.88)

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  $\geq 3$ , 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	202	
1	B	202	
1	C	202	
1	D	202	
2	E	229	

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Mol	Chain	Length	Quality of chain
2	H	229	 3% 83% 14% ..
2	J	229	 3% 82% 15% ..
2	M	229	 3% 86% 11% ..
3	F	214	 3% 86% 13% .
3	K	214	 4% 86% 11% ..
3	L	214	 0% 87% 11% .
3	N	214	 4% 91% 7% .
4	O	222	 1% 84% 13% .
4	Q	222	 1% 81% 16% .
4	S	222	 1% 84% 13% .
4	X	222	 2% 84% 13% .
5	P	216	 1% 85% 13% .
5	R	216	 2% 89% 10% .
5	T	216	 4% 86% 12% .
5	Y	216	 1% 90% 9% .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31966 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 S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	195	1557	1001	264	284	8	0	0	0
1	B	194	1550	997	263	282	8	0	0	0
1	C	195	1551	998	262	283	8	0	0	0
1	A	195	1556	1001	264	283	8	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	327	HIS	-	expression tag	UNP P0DTC2
D	328	HIS	-	expression tag	UNP P0DTC2
D	329	HIS	-	expression tag	UNP P0DTC2
D	330	HIS	-	expression tag	UNP P0DTC2
D	331	HIS	-	expression tag	UNP P0DTC2
D	332	HIS	-	expression tag	UNP P0DTC2
D	339	ASP	GLY	variant	UNP P0DTC2
D	371	LEU	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	446	SER	GLY	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	493	ARG	GLN	variant	UNP P0DTC2
D	496	SER	GLY	variant	UNP P0DTC2
D	498	ARG	GLN	conflict	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	527	LYS	-	expression tag	UNP P0DTC2
D	528	LYS	-	expression tag	UNP P0DTC2
B	327	HIS	-	expression tag	UNP P0DTC2
B	328	HIS	-	expression tag	UNP P0DTC2
B	329	HIS	-	expression tag	UNP P0DTC2
B	330	HIS	-	expression tag	UNP P0DTC2
B	331	HIS	-	expression tag	UNP P0DTC2
B	332	HIS	-	expression tag	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	527	LYS	-	expression tag	UNP P0DTC2
B	528	LYS	-	expression tag	UNP P0DTC2
C	327	HIS	-	expression tag	UNP P0DTC2
C	328	HIS	-	expression tag	UNP P0DTC2
C	329	HIS	-	expression tag	UNP P0DTC2
C	330	HIS	-	expression tag	UNP P0DTC2
C	331	HIS	-	expression tag	UNP P0DTC2
C	332	HIS	-	expression tag	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	527	LYS	-	expression tag	UNP P0DTC2
C	528	LYS	-	expression tag	UNP P0DTC2
A	327	HIS	-	expression tag	UNP P0DTC2
A	328	HIS	-	expression tag	UNP P0DTC2
A	329	HIS	-	expression tag	UNP P0DTC2
A	330	HIS	-	expression tag	UNP P0DTC2
A	331	HIS	-	expression tag	UNP P0DTC2
A	332	HIS	-	expression tag	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	527	LYS	-	expression tag	UNP P0DTC2
A	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Omi-6 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	224	Total	C	N	O	S	0	0	0
			1605	1006	269	323	7			
2	M	224	Total	C	N	O	S	0	0	0
			1615	1015	270	323	7			
2	J	224	Total	C	N	O	S	0	0	0
			1608	1010	269	322	7			
2	H	224	Total	C	N	O	S	0	0	0
			1615	1015	270	323	7			

- Molecule 3 is a protein called Omi-6 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	212	Total	C	N	O	S	0	0	0
			1603	998	273	327	5			
3	K	211	Total	C	N	O	S	0	0	0
			1592	994	268	325	5			
3	N	210	Total	C	N	O	S	0	0	0
			1581	986	267	323	5			
3	L	211	Total	C	N	O	S	0	0	0
			1604	1002	272	325	5			

- Molecule 4 is a protein called COVOX-150 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	215	Total	C	N	O	S	0	0	0
			1592	1002	265	316	9			
4	S	215	Total	C	N	O	S	0	0	0
			1592	1002	265	316	9			
4	O	214	Total	C	N	O	S	0	0	0
			1583	997	263	314	9			
4	Q	215	Total	C	N	O	S	0	0	0
			1592	1002	265	316	9			

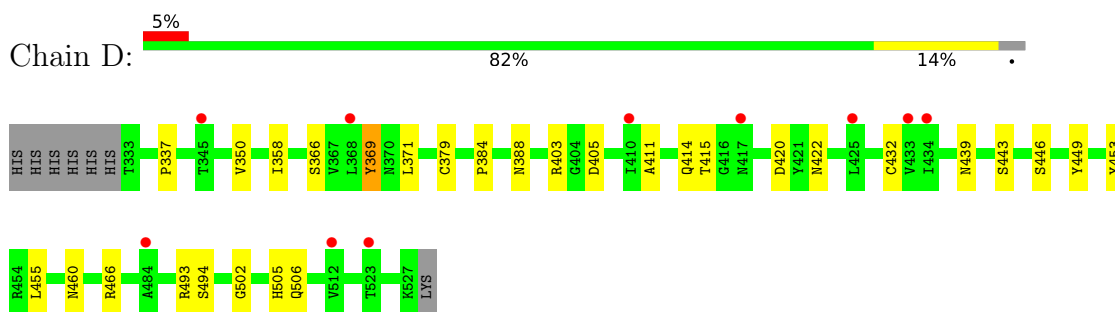
- Molecule 5 is a protein called COVOX-150 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Y	215	Total	C	N	O	S	0	1	0
			1646	1034	272	335	5			
5	T	215	Total	C	N	O	S	0	1	0
			1643	1033	272	333	5			
5	P	214	Total	C	N	O	S	0	1	0
			1635	1028	268	334	5			
5	R	215	Total	C	N	O	S	0	1	0
			1646	1034	272	335	5			

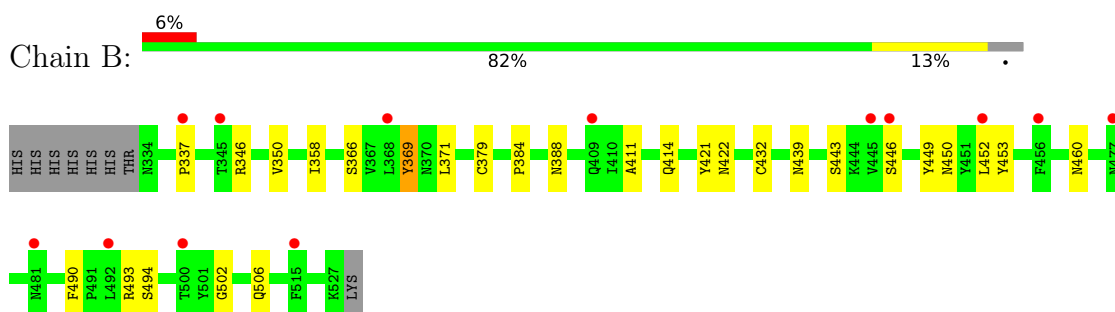
### 3 Residue-property plots [i](#)

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.

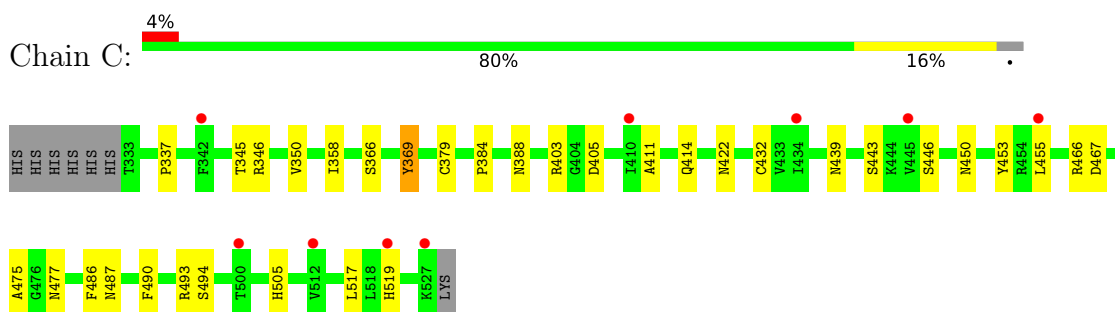
- Molecule 1: Spike protein S1



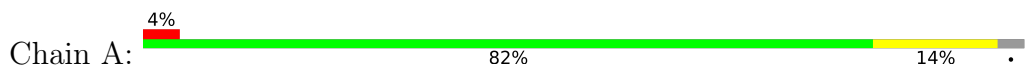
- Molecule 1: Spike protein S1

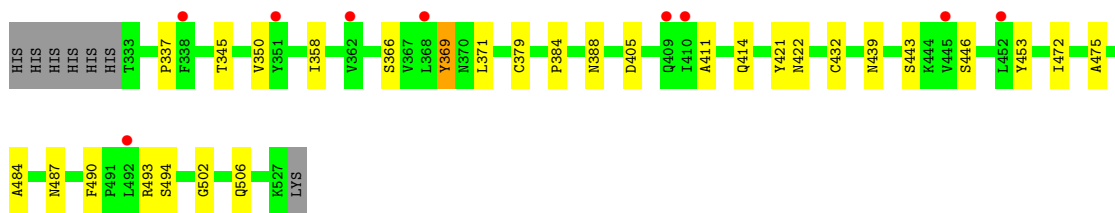


- Molecule 1: Spike protein S1

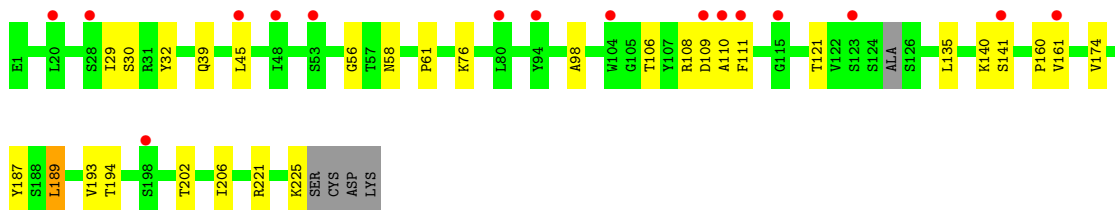
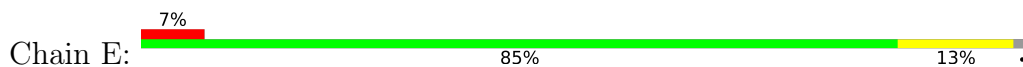


- Molecule 1: Spike protein S1

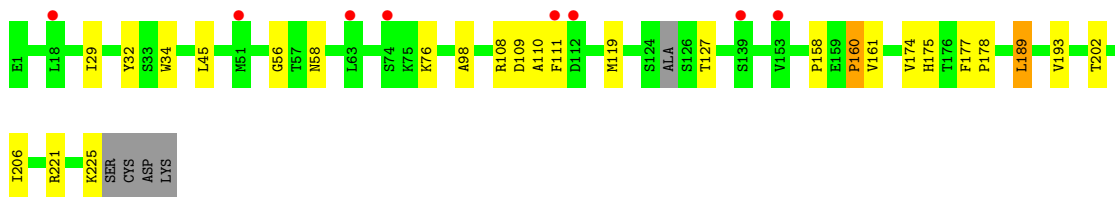
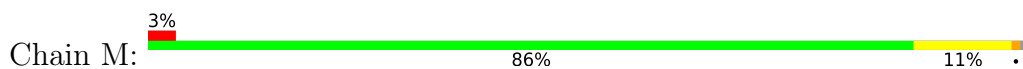




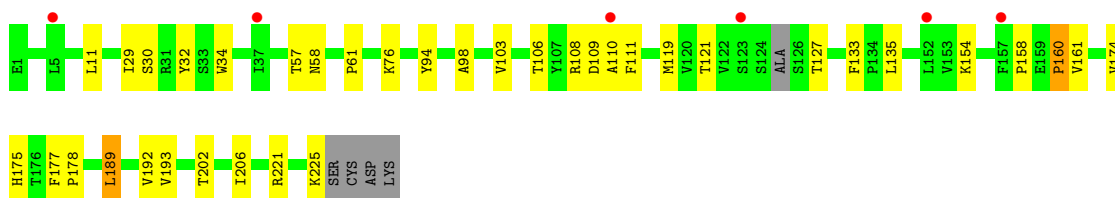
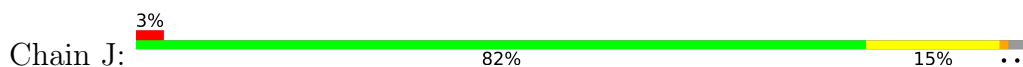
- Molecule 2: Omi-6 heavy chain



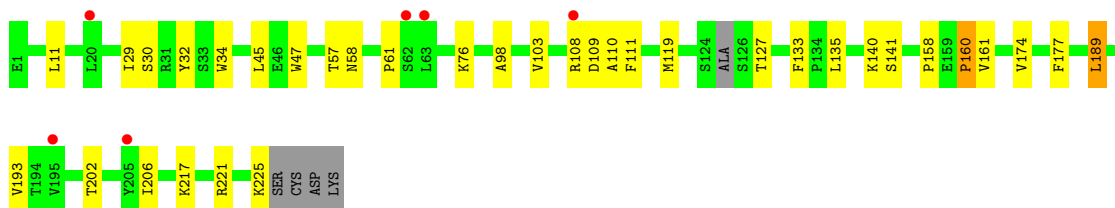
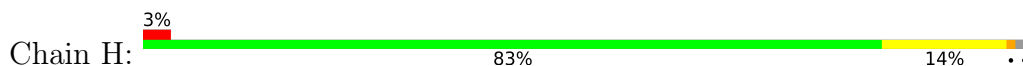
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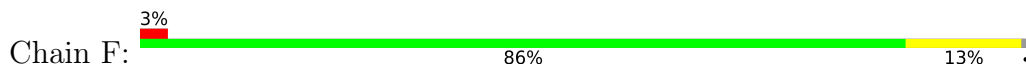
- Molecule 2: Omi-6 heavy chain



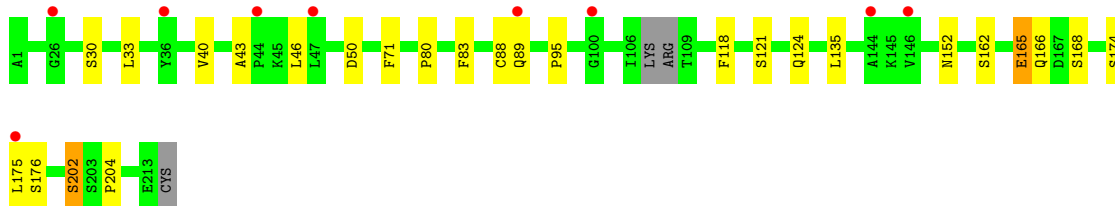
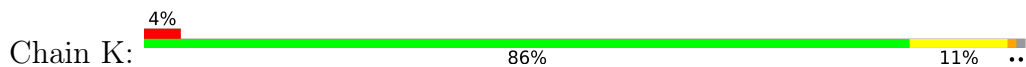
- Molecule 2: Omi-6 heavy chain



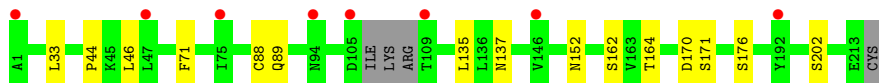
- Molecule 3: Omi-6 light chain



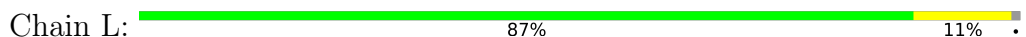
- Molecule 3: Omi-6 light chain



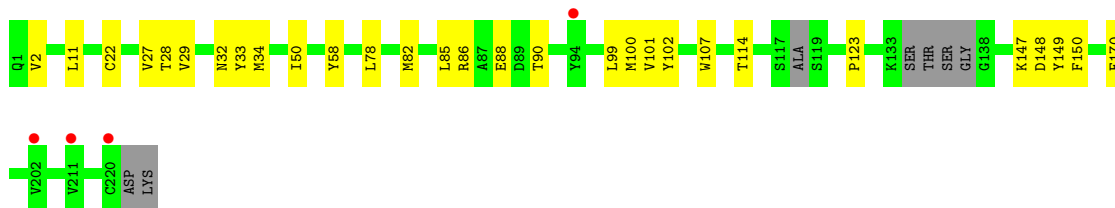
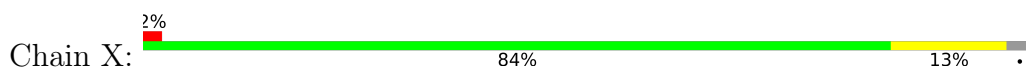
- Molecule 3: Omi-6 light chain



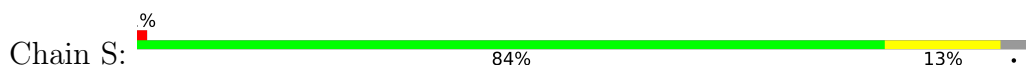
- Molecule 3: Omi-6 light chain

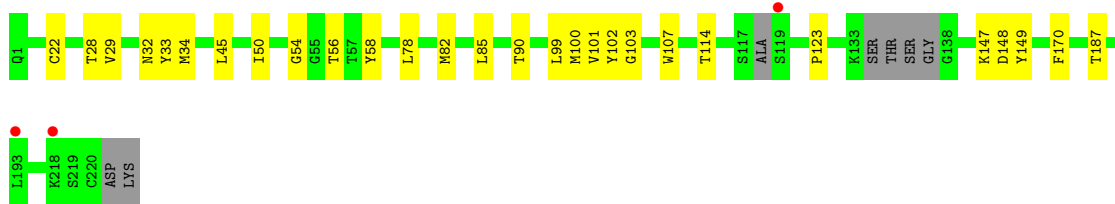


- Molecule 4: COVOX-150 heavy chain

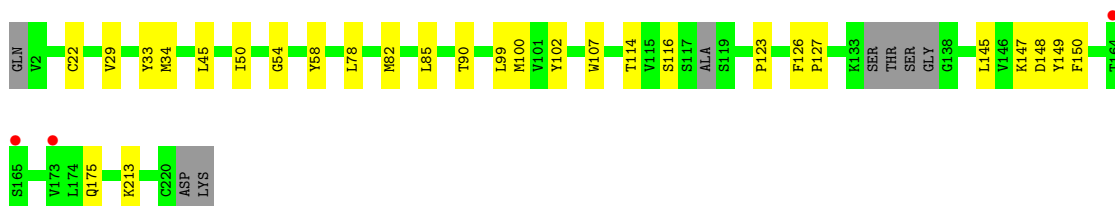
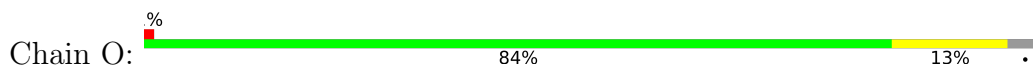


- Molecule 4: COVOX-150 heavy chain

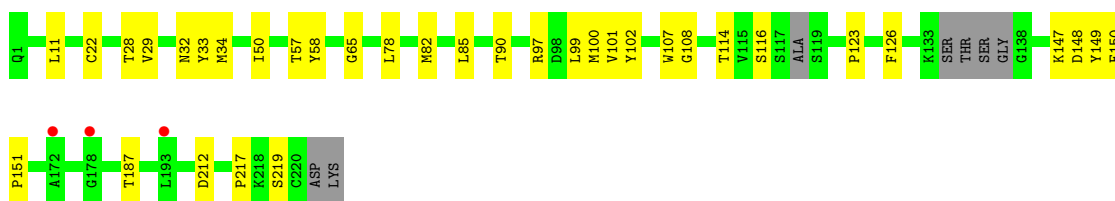
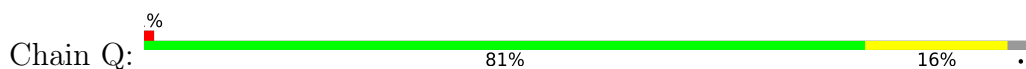




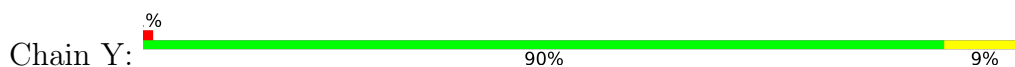
- Molecule 4: COVOX-150 heavy chain



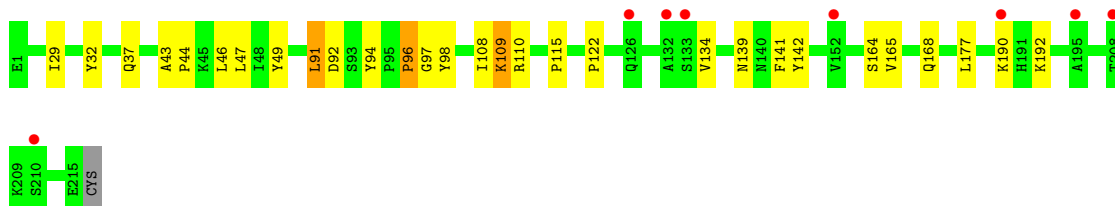
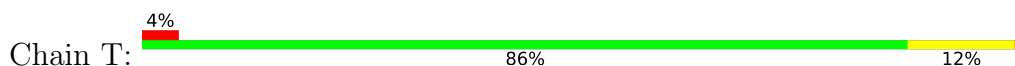
- Molecule 4: COVOX-150 heavy chain



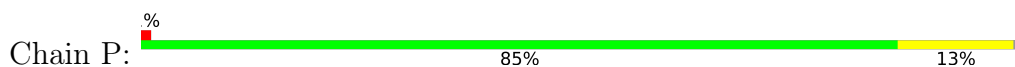
- Molecule 5: COVOX-150 light chain

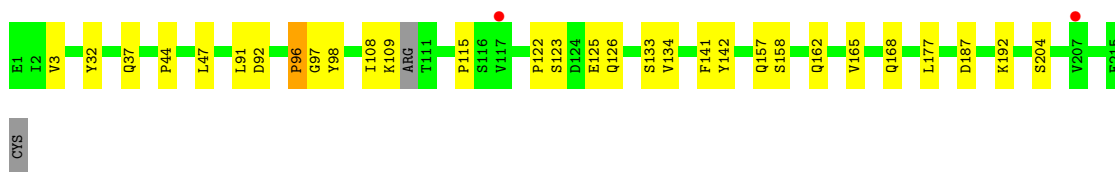


- Molecule 5: COVOX-150 light chain



- Molecule 5: COVOX-150 light chain

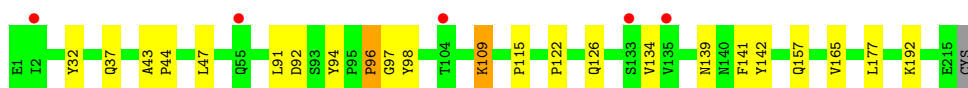




CYS

- Molecule 5: COVOX-150 light chain

Chain R: 2% 89% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.82Å 114.78Å 144.55Å 82.01° 80.62° 86.17°	Depositor
Resolution (Å)	113.55 – 4.24 113.55 – 4.24	Depositor EDS
% Data completeness (in resolution range)	34.0 (113.55-4.24) 34.0 (113.55-4.24)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 4.30Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.237 , 0.272 0.235 , 0.273	Depositor DCC
$R_{free}$ test set	595 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 97.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	31966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.10	0/1601	0.23	0/2179
1	B	0.10	0/1595	0.23	0/2171
1	C	0.10	0/1595	0.24	0/2171
1	D	0.10	0/1602	0.23	0/2181
2	E	0.57	0/1639	0.85	0/2238
2	H	0.57	0/1650	0.86	0/2251
2	J	0.57	0/1643	0.85	0/2242
2	M	0.57	0/1650	0.86	0/2251
3	F	0.56	0/1634	0.86	0/2215
3	K	0.56	0/1624	0.85	0/2203
3	L	0.56	0/1637	0.85	0/2219
3	N	0.56	0/1613	0.88	1/2188 (0.0%)
4	O	0.09	0/1616	0.26	0/2201
4	Q	0.09	0/1625	0.26	0/2213
4	S	0.09	0/1625	0.26	0/2213
4	X	0.09	0/1625	0.26	0/2213
5	P	0.11	0/1673	0.32	0/2273
5	R	0.11	0/1685	0.61	3/2290 (0.1%)
5	T	0.24	2/1682 (0.1%)	0.36	0/2286
5	Y	0.14	0/1685	0.66	3/2290 (0.1%)
All	All	0.37	2/32699 (0.0%)	0.61	7/44488 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	110	ARG	N-CA	6.27	1.53	1.46
5	T	109	LYS	CA-C	6.09	1.60	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	109	LYS	O-C-N	19.70	146.26	123.01
5	R	109	LYS	O-C-N	-15.82	104.34	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	109	LYS	CA-C-N	-13.65	100.41	122.11
5	Y	109	LYS	C-N-CA	-13.65	100.41	122.11
5	R	109	LYS	CA-C-N	13.57	143.69	122.11

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	1556	0	1482	37	0
1	B	1550	0	1475	30	0
1	C	1551	0	1477	48	0
1	D	1557	0	1482	38	0
2	E	1605	0	1546	50	0
2	H	1615	0	1564	44	2
2	J	1608	0	1549	74	0
2	M	1615	0	1564	29	0
3	F	1603	0	1554	47	1
3	K	1592	0	1532	60	2
3	L	1604	0	1553	37	0
3	N	1581	0	1520	16	0
4	O	1583	0	1555	45	0
4	Q	1592	0	1567	31	2
4	S	1592	0	1567	35	0
4	X	1592	0	1567	25	0
5	P	1635	0	1593	50	0
5	R	1646	0	1607	26	0
5	T	1643	0	1605	36	1
5	Y	1646	0	1607	16	0
All	All	31966	0	30966	510	4

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.

The worst 5 of 510 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:449:TYR:CE2	2:M:56:GLY:HA3	1.61	1.35
4:O:213:LYS:NZ	5:P:125:GLU:OE1	1.58	1.33
1:D:449:TYR:CZ	2:M:56:GLY:HA3	1.65	1.32
4:O:126:PHE:CZ	5:P:126:GLN:HG3	1.72	1.24
3:K:46:LEU:CD2	2:J:110:ALA:HB1	1.66	1.24

All (4) 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)
3:F:188:LYS:O	2:H:217:LYS:N[1_565]	1.99	0.21
3:K:204:PRO:CG	4:Q:65:GLY:O[1_554]	2.10	0.10
5:T:190:LYS:NZ	2:H:103:VAL:O[1_655]	2.10	0.10
3:K:202:SER:OG	4:Q:57:THR:OG1[1_554]	2.19	0.01

## 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	193/202 (96%)	179 (93%)	14 (7%)	0	100	100
1	B	192/202 (95%)	178 (93%)	14 (7%)	0	100	100
1	C	193/202 (96%)	179 (93%)	14 (7%)	0	100	100
1	D	193/202 (96%)	179 (93%)	14 (7%)	0	100	100
2	E	220/229 (96%)	209 (95%)	9 (4%)	2 (1%)	14	49
2	H	220/229 (96%)	209 (95%)	9 (4%)	2 (1%)	14	49
2	J	220/229 (96%)	209 (95%)	9 (4%)	2 (1%)	14	49
2	M	220/229 (96%)	209 (95%)	9 (4%)	2 (1%)	14	49
3	F	208/214 (97%)	202 (97%)	6 (3%)	0	100	100
3	K	207/214 (97%)	201 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	207/214 (97%)	201 (97%)	6 (3%)	0	100	100
3	N	206/214 (96%)	199 (97%)	7 (3%)	0	100	100
4	O	208/222 (94%)	202 (97%)	6 (3%)	0	100	100
4	Q	209/222 (94%)	203 (97%)	6 (3%)	0	100	100
4	S	209/222 (94%)	203 (97%)	6 (3%)	0	100	100
4	X	209/222 (94%)	203 (97%)	6 (3%)	0	100	100
5	P	211/216 (98%)	200 (95%)	9 (4%)	2 (1%)	14	49
5	R	214/216 (99%)	203 (95%)	9 (4%)	2 (1%)	14	49
5	T	214/216 (99%)	203 (95%)	9 (4%)	2 (1%)	14	49
5	Y	214/216 (99%)	203 (95%)	9 (4%)	2 (1%)	14	49
All	All	4167/4332 (96%)	3974 (95%)	177 (4%)	16 (0%)	30	66

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	109	ASP
2	M	109	ASP
5	Y	96	PRO
5	T	96	PRO
5	P	96	PRO

### 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	168/177 (95%)	167 (99%)	1 (1%)	78	80
1	B	167/177 (94%)	166 (99%)	1 (1%)	78	80
1	C	167/177 (94%)	166 (99%)	1 (1%)	78	80
1	D	168/177 (95%)	167 (99%)	1 (1%)	78	80
2	E	176/195 (90%)	172 (98%)	4 (2%)	44	63
2	H	178/195 (91%)	174 (98%)	4 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	176/195 (90%)	172 (98%)	4 (2%)	44	63
2	M	178/195 (91%)	174 (98%)	4 (2%)	45	64
3	F	181/185 (98%)	179 (99%)	2 (1%)	65	73
3	K	178/185 (96%)	175 (98%)	3 (2%)	53	67
3	L	181/185 (98%)	179 (99%)	2 (1%)	65	73
3	N	177/185 (96%)	175 (99%)	2 (1%)	65	73
4	O	180/187 (96%)	180 (100%)	0	100	100
4	Q	181/187 (97%)	181 (100%)	0	100	100
4	S	181/187 (97%)	181 (100%)	0	100	100
4	X	181/187 (97%)	181 (100%)	0	100	100
5	P	187/188 (100%)	185 (99%)	2 (1%)	65	73
5	R	188/188 (100%)	186 (99%)	2 (1%)	65	73
5	T	187/188 (100%)	185 (99%)	2 (1%)	65	73
5	Y	188/188 (100%)	186 (99%)	2 (1%)	65	73
All	All	3568/3728 (96%)	3531 (99%)	37 (1%)	68	75

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	R	192	LYS
2	H	202	THR
2	J	160	PRO
2	J	225	LYS
3	K	202	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
4	X	83	ASN
2	H	39	GLN
5	T	55	GLN
2	H	175	HIS
2	J	77	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	195/202 (96%)	0.32	9 (4%) 37 32	81, 115, 197, 235	0
1	B	194/202 (96%)	0.35	13 (6%) 24 24	64, 120, 185, 206	0
1	C	195/202 (96%)	0.25	9 (4%) 37 32	66, 113, 150, 188	0
1	D	195/202 (96%)	0.37	10 (5%) 33 30	76, 115, 219, 240	0
2	E	224/229 (97%)	0.44	16 (7%) 22 23	60, 101, 142, 166	0
2	H	224/229 (97%)	0.27	6 (2%) 56 43	75, 112, 135, 165	0
2	J	224/229 (97%)	0.34	6 (2%) 56 43	62, 122, 163, 199	0
2	M	224/229 (97%)	0.22	8 (3%) 46 37	62, 105, 140, 196	0
3	F	212/214 (99%)	0.21	7 (3%) 49 39	69, 108, 142, 186	0
3	K	211/214 (98%)	0.13	9 (4%) 40 34	79, 132, 169, 188	0
3	L	211/214 (98%)	0.08	1 (0%) 87 75	77, 108, 142, 166	0
3	N	210/214 (98%)	0.33	8 (3%) 44 36	57, 118, 154, 172	0
4	O	214/222 (96%)	0.02	3 (1%) 73 57	56, 94, 124, 138	0
4	Q	215/222 (96%)	0.07	3 (1%) 73 57	53, 87, 115, 134	0
4	S	215/222 (96%)	0.07	3 (1%) 73 57	58, 94, 117, 145	0
4	X	215/222 (96%)	0.04	4 (1%) 66 51	54, 89, 116, 181	0
5	P	214/216 (99%)	-0.03	2 (0%) 81 66	55, 91, 113, 122	1 (0%)
5	R	215/216 (99%)	0.03	5 (2%) 61 47	36, 90, 120, 148	1 (0%)
5	T	215/216 (99%)	0.07	8 (3%) 45 36	51, 93, 120, 138	1 (0%)
5	Y	215/216 (99%)	0.10	2 (0%) 81 66	59, 95, 120, 142	1 (0%)
All	All	4237/4332 (97%)	0.18	132 (3%) 51 40	36, 104, 151, 240	4 (0%)

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	VAL	6.1
1	D	345	THR	6.1
2	E	110	ALA	5.5
3	F	44	PRO	5.3
2	H	205	TYR	4.8

## 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.