



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8YDL / pdb_00008ydl
Title : Crystal structure of single-chain dimer for RSV F protein
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Deposited on : 2024-02-20
Resolution : 2.60 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

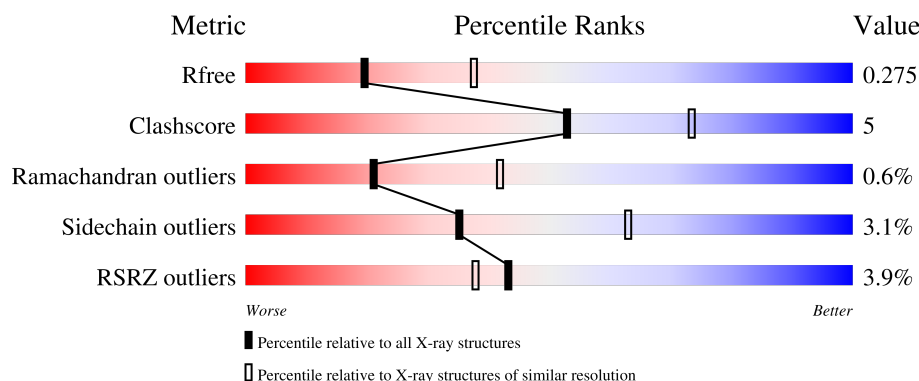
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	491	4% 77% 13% • 9%
1	B	491	3% 76% 14% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7090 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 Fusion glycoprotein F2, F1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	4	0
			3456	2190	574	670	22			
1	B	446	Total	C	N	O	S	0	5	0
			3461	2193	575	671	22			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total	O	0	0
			89	89		
2	B	84	Total	O	0	0
			84	84		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.66Å 59.91Å 102.42Å 76.38° 73.70° 76.77°	Depositor
Resolution (Å)	46.44 – 2.60 46.44 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.9 (46.44-2.60) 86.0 (46.44-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.234 , 0.265 0.245 , 0.275	Depositor DCC
R_{free} test set	1880 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.118 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7090	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 98.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6076e-11. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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	0.20	0/3504	0.42	2/4746 (0.0%)
1	B	0.20	0/3512	0.41	2/4757 (0.0%)
All	All	0.20	0/7016	0.42	4/9503 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ALA	CA-C-N	-5.93	113.24	122.37
1	B	47	ALA	C-N-CA	-5.93	113.24	122.37
1	A	288	SER	CA-C-N	-5.87	112.77	122.39
1	A	288	SER	C-N-CA	-5.87	112.77	122.39

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	3456	0	3628	34	0
1	B	3461	0	3634	38	0
2	A	89	0	0	1	0
2	B	84	0	0	3	0
All	All	7090	0	7262	71	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 5.

All (71) 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:B:77:LYS:O	1:B:81:GLN:HG3	1.89	0.72
1:A:46:SER:HB3	1:A:245:GLN:HE22	1.54	0.71
1:A:228:THR:HB	1:A:231:GLN:HG3	1.77	0.66
1:A:46:SER:CB	1:A:245:GLN:HE22	2.09	0.65
1:B:379:LYS:HE3	2:B:673:HOH:O	1.96	0.65
1:A:46:SER:C	1:A:48:LEU:H	2.08	0.62
1:A:228:THR:HG22	1:A:231:GLN:H	1.64	0.61
1:A:240:GLN:H	1:A:240:GLN:CD	2.09	0.60
1:A:460:LEU:HD23	1:A:481:VAL:HG13	1.86	0.58
1:B:336:GLN:O	1:B:340:GLN:HG3	2.04	0.57
1:B:227:ILE:HG13	1:B:232:LYS:HG3	1.85	0.57
1:B:482:GLN:NE2	2:B:601:HOH:O	2.29	0.56
1:A:319:LYS:O	1:A:323:GLN:HG3	2.06	0.56
1:B:240:GLN:H	1:B:240:GLN:CD	2.14	0.56
1:A:228:THR:HG23	2:A:660:HOH:O	2.05	0.55
1:B:460:LEU:HD23	1:B:481:VAL:HG13	1.89	0.55
1:B:302:GLU:HB2	1:B:397:ASP:HA	1.90	0.54
1:B:319:LYS:O	1:B:323:GLN:HG3	2.08	0.54
1:A:235:MET:HE2	1:A:267:TYR:HD2	1.72	0.53
1:A:77:LYS:O	1:A:81:GLN:HG3	2.08	0.53
1:A:471:ASN:OD1	1:B:136:ASN:ND2	2.42	0.53
1:A:336:GLN:O	1:A:340:GLN:HG3	2.09	0.52
1:B:315:ASP:OD2	1:B:317:LYS:NZ	2.42	0.52
1:A:304:SER:HB2	1:A:399:LYS:HA	1.92	0.52
1:A:93:LEU:O	1:A:97:MET:HG3	2.10	0.52
1:B:335:LEU:HG	1:B:437:THR:HG23	1.93	0.51
1:A:235:MET:HE2	1:A:267:TYR:CD2	2.47	0.50
1:A:61:LEU:HD11	1:A:258:LEU:HB2	1.94	0.50
1:A:106:GLY:O	1:A:291:ARG:NH1	2.40	0.49
1:A:228:THR:CB	1:A:231:GLN:HG3	2.43	0.48
1:A:171:GLN:HB2	1:A:174:SER:OG	2.14	0.48
1:B:171:GLN:HB2	1:B:174:SER:OG	2.13	0.48
1:B:235:MET:HE2	1:B:267:TYR:CD2	2.49	0.48
1:B:321:ILE:HD11	1:B:423:VAL:HA	1.95	0.47
1:B:64:ILE:HD12	1:B:165:LEU:HD11	1.95	0.47
1:B:228:THR:OG1	1:B:231:GLN:HG3	2.14	0.47
1:A:483:ILE:O	1:A:487:GLN:HG2	2.15	0.46
1:A:411:ASN:O	1:A:412:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:CG2	1:A:230:ASP:H	2.29	0.46
1:A:470:THR:OG1	1:A:473:GLN:HG3	2.16	0.46
1:B:235:MET:HE2	1:B:267:TYR:HD2	1.82	0.45
1:B:304:SER:HB2	1:B:399:LYS:HA	1.98	0.45
1:A:228:THR:HG23	1:A:230:ASP:H	1.82	0.45
1:B:303:LEU:O	1:B:399:LYS:HB2	2.16	0.45
1:B:73:ASP:O	1:B:77:LYS:HG3	2.17	0.45
1:A:64:ILE:O	1:A:64:ILE:HG13	2.17	0.44
1:B:483:ILE:O	1:B:487:GLN:HG2	2.17	0.44
1:A:420:ILE:O	1:A:424:ILE:HG12	2.17	0.44
1:B:305:ASN:N	2:B:603:HOH:O	2.49	0.44
1:B:311:CYS:HB2	1:B:414:SER:HA	1.98	0.44
1:A:158:ASN:O	1:A:162:LYS:HB2	2.17	0.44
1:B:160:ILE:HA	1:B:164:LEU:HB3	1.99	0.44
1:B:82:GLU:HA	1:B:85:LYS:HD2	1.99	0.44
1:A:335:LEU:HG	1:A:437:THR:HG23	2.01	0.43
1:B:60:GLU:HB2	1:B:155:ASP:HA	2.00	0.43
1:B:470:THR:OG1	1:B:473:GLN:HG3	2.18	0.43
1:B:298:VAL:HB	1:B:392:THR:HG22	2.01	0.43
1:B:494:ILE:HD11	1:B:496:LYS:HD3	2.00	0.43
1:A:421:GLU:OE1	1:A:421:GLU:N	2.39	0.42
1:B:303:LEU:HD11	1:B:500:LEU:HB2	2.01	0.42
1:B:463:LEU:HD22	1:B:506:LEU:HD22	2.00	0.42
1:A:504:VAL:HG12	1:A:506:LEU:CD1	2.50	0.42
1:B:46:SER:CB	1:B:245:GLN:HE22	2.33	0.41
1:B:221:LEU:HD22	1:B:264:LEU:HD22	2.01	0.41
1:A:430:ASN:O	1:A:434:LEU:HG	2.21	0.41
1:B:66:GLU:H	1:B:66:GLU:HG2	1.71	0.41
1:B:312:ASN:HB2	1:B:414:SER:HB3	2.03	0.41
1:A:221:LEU:HD22	1:A:264:LEU:HD22	2.02	0.41
1:B:178:ILE:O	1:B:182:ILE:HG12	2.21	0.41
1:A:227:ILE:HG13	1:A:232:LYS:HG3	2.03	0.40
1:B:504:VAL:HG12	1:B:506:LEU:CD1	2.51	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	446/491 (91%)	433 (97%)	10 (2%)	3 (1%)	18	38
1	B	447/491 (91%)	432 (97%)	13 (3%)	2 (0%)	30	51
All	All	893/982 (91%)	865 (97%)	23 (3%)	5 (1%)	21	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	LYS
1	A	413	GLN
1	B	412	LYS
1	B	413	GLN
1	A	47	ALA

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	410/445 (92%)	393 (96%)	17 (4%)	27	54
1	B	411/445 (92%)	403 (98%)	8 (2%)	50	75
All	All	821/890 (92%)	796 (97%)	25 (3%)	35	64

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS

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Mol	Chain	Res	Type
1	A	95	LEU
1	A	99	SER
1	A	134	SER
1	A	173	CYS
1	A	174	SER
1	A	228	THR
1	A	262	VAL
1	A	329	LYS
1	A	364	GLU
1	A	372	SER
1	A	374	LEU
1	A	376	SER
1	A	400	ASN
1	A	405	GLN
1	A	415	CYS
1	A	465	ASN
1	B	46	SER
1	B	64	ILE
1	B	99	SER
1	B	173	CYS
1	B	400	ASN
1	B	412	LYS
1	B	415	CYS
1	B	448	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	245	GLN
1	A	340	GLN
1	A	465	ASN
1	A	486	GLN
1	B	223	ASN
1	B	323	GLN
1	B	471	ASN
1	B	473	GLN
1	B	482	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 ⓘ

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	446/491 (90%)	-0.99	20 (4%) 38 32	9, 38, 103, 194	4 (0%)
1	B	446/491 (90%)	-0.98	15 (3%) 48 42	13, 38, 110, 208	5 (1%)
All	All	892/982 (90%)	-0.99	35 (3%) 43 38	9, 38, 111, 208	9 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	413	GLN	4.9
1	B	346	GLY	4.5
1	A	343	PRO	4.0
1	B	344	ALA	3.5
1	B	316	ALA	3.5
1	B	348	GLY	3.3
1	A	413	GLN	3.2
1	A	414	SER	3.2
1	A	72	THR	3.0
1	B	311	CYS	3.0
1	A	100	THR	2.9
1	A	345	THR	2.9
1	B	410	LEU	2.8
1	A	346	GLY	2.7
1	A	348	GLY	2.7
1	A	347	SER	2.6
1	B	70	ASN	2.6
1	B	100	THR	2.5
1	A	342	THR	2.4
1	A	410	LEU	2.4
1	A	73	ASP	2.4
1	A	171	GLN	2.4
1	A	344	ALA	2.4
1	B	72	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	313	GLY	2.3
1	B	345	THR	2.2
1	A	311	CYS	2.2
1	A	418	PRO	2.2
1	A	315	ASP	2.1
1	B	73	ASP	2.1
1	B	414	SER	2.1
1	B	315	ASP	2.1
1	A	312	ASN	2.1
1	A	316	ALA	2.0
1	B	343	PRO	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.