



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2021 – 10:35 AM EDT

PDB ID : 7RK2
Title : Crystal structure of the human astrovirus serotype 8 capsid spike in complex with scFv 2D9, an astrovirus-neutralizing antibody, at 2.65-Å resolution
Authors : Meyer, L.; Cuellar, C.; DuBois, R.M.
Deposited on : 2021-07-21
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

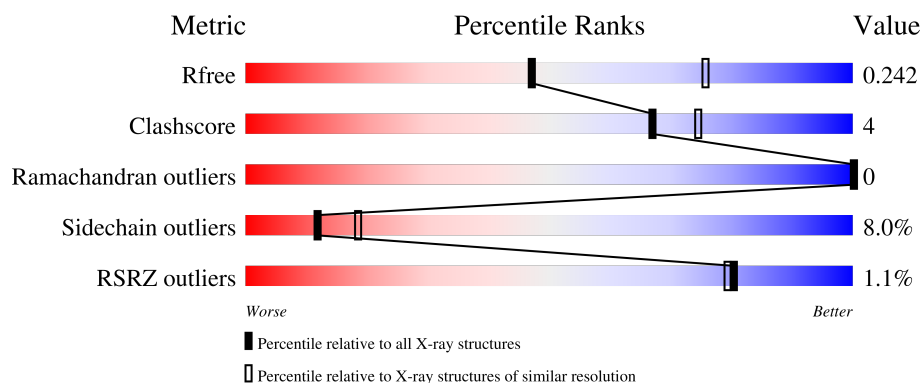
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	230	 81% 13% 6%
1	B	230	 80% 15% 5%
2	C	251	 72% 17% 11%
2	D	251	 71% 18% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7106 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 Capsid protein VP25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1740	1113	292	329	6			
1	B	218	Total	C	N	O	S	0	1	0
			1754	1121	296	331	6			

There are 22 discrepancies between the modelled and reference sequences:

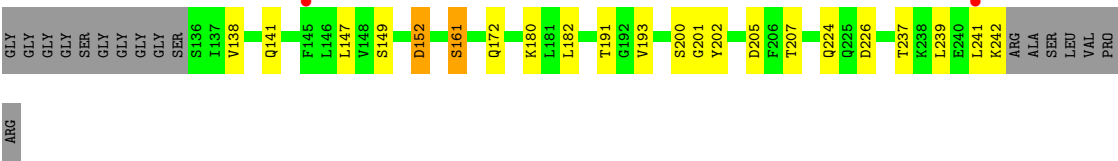
Chain	Residue	Modelled	Actual	Comment	Reference
A	427	MET	-	initiating methionine	UNP Q9IFX1
A	428	GLY	-	expression tag	UNP Q9IFX1
A	648	ALA	-	expression tag	UNP Q9IFX1
A	649	ALA	-	expression tag	UNP Q9IFX1
A	650	GLU	-	expression tag	UNP Q9IFX1
A	651	LEU	-	expression tag	UNP Q9IFX1
A	652	ALA	-	expression tag	UNP Q9IFX1
A	653	LEU	-	expression tag	UNP Q9IFX1
A	654	VAL	-	expression tag	UNP Q9IFX1
A	655	PRO	-	expression tag	UNP Q9IFX1
A	656	ARG	-	expression tag	UNP Q9IFX1
B	427	MET	-	initiating methionine	UNP Q9IFX1
B	428	GLY	-	expression tag	UNP Q9IFX1
B	648	ALA	-	expression tag	UNP Q9IFX1
B	649	ALA	-	expression tag	UNP Q9IFX1
B	650	GLU	-	expression tag	UNP Q9IFX1
B	651	LEU	-	expression tag	UNP Q9IFX1
B	652	ALA	-	expression tag	UNP Q9IFX1
B	653	LEU	-	expression tag	UNP Q9IFX1
B	654	VAL	-	expression tag	UNP Q9IFX1
B	655	PRO	-	expression tag	UNP Q9IFX1
B	656	ARG	-	expression tag	UNP Q9IFX1

- Molecule 2 is a protein called scFv 2D9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	224	Total 1731	C 1101	N 285	O 338	S 7	0	1	0
2	D	224	Total 1731	C 1101	N 285	O 338	S 7	0	1	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total 46	O 46	0	0
3	B	39	Total 39	O 39	0	0
3	C	44	Total 44	O 44	0	0
3	D	21	Total 21	O 21	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.59Å 97.34Å 208.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	104.15 – 2.65 104.15 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (104.15-2.65) 99.9 (104.15-2.65)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.218 , 0.247 0.212 , 0.242	Depositor DCC
R_{free} test set	1998 reflections (6.61%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7106	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 34.75 % 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 6.4997e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.61	0/1793	0.76	0/2457
1	B	0.69	0/1808	0.73	0/2477
2	C	0.64	0/1771	0.75	0/2406
2	D	0.61	0/1771	0.69	0/2406
All	All	0.64	0/7143	0.73	0/9746

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
2	C	0	3
2	D	0	4
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	201	GLY	Mainchain
2	C	202[A]	TYR	Mainchain
2	D	201	GLY	Mainchain
2	D	202[A]	TYR	Mainchain
2	D	202[B]	TYR	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	1740	0	1680	14	0
1	B	1754	0	1689	13	0
2	C	1731	0	1685	12	0
2	D	1731	0	1685	15	0
3	A	46	0	0	1	0
3	B	39	0	0	1	0
3	C	44	0	0	1	0
3	D	21	0	0	0	0
All	All	7106	0	6739	53	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 4.

All (53) 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:438:VAL:HG11	1:A:630:PRO:HG2	1.80	0.61
2:D:172:GLN:HB2	2:D:182:LEU:HD11	1.82	0.61
1:A:437:THR:HG23	1:A:633:ALA:HA	1.83	0.59
1:B:438:VAL:HG11	1:B:630:PRO:HG2	1.85	0.58
1:B:620:ASP:OD1	1:B:623:MET:HG3	2.04	0.58
2:C:40:SER:HB2	2:C:43:LYS:HB2	1.85	0.57
1:A:456:THR:HB	3:A:702:HOH:O	2.05	0.56
1:A:538:VAL:HG12	1:A:591:THR:HG22	1.89	0.55
1:B:444:PRO:HG3	1:B:578:THR:HG21	1.88	0.55
2:D:38:ARG:HD3	2:D:48:LEU:HD21	1.90	0.54
2:D:224:GLN:NE2	2:D:226:ASP:HB2	2.23	0.53
1:B:508:ALA:HB3	1:B:516:ALA:HB3	1.91	0.53
2:D:51:ILE:HG13	2:D:57:THR:HG22	1.91	0.52
1:A:450:GLN:HG3	1:A:555:TYR:CG	2.47	0.50
2:D:138:VAL:H	2:D:161:SER:HB3	1.76	0.50
2:C:82:MET:HE3	2:C:85:LEU:HD11	1.94	0.50
1:B:456:THR:HB	3:B:720:HOH:O	2.12	0.49
1:B:542:ARG:HE	1:B:585:GLY:HA2	1.77	0.49
2:D:141:GLN:NE2	2:D:237:THR:OG1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:SER:O	2:D:152:ASP:HB2	2.13	0.48
2:C:90:THR:HG23	2:C:114:THR:HA	1.96	0.47
1:A:459:PRO:HB3	1:A:465:THR:HG23	1.97	0.47
2:C:72:ASP:HB3	2:C:75:LYS:HG2	1.96	0.47
2:C:218:LEU:HD11	2:C:241:LEU:HB2	1.97	0.47
1:B:429:GLY:N	1:B:641:HIS:HD1	2.14	0.46
1:A:436:LEU:HD21	1:A:484:VAL:HG22	1.97	0.46
2:D:239:LEU:HD12	2:D:239:LEU:HA	1.73	0.46
1:A:583:THR:HB	1:A:586:LYS:HG3	1.97	0.46
1:B:548:GLN:HG3	1:B:581:GLN:HG2	1.97	0.46
1:A:618:ARG:HD3	1:B:631:PRO:HG3	1.99	0.44
1:A:435:LEU:HA	1:A:435:LEU:HD23	1.72	0.44
2:D:182:LEU:HA	2:D:193:VAL:HG21	1.98	0.44
2:C:48:LEU:HB3	2:C:67:LEU:HD11	1.99	0.43
2:C:193:VAL:HA	2:C:194:PRO:HD3	1.74	0.43
1:A:434:VAL:HG22	1:A:638:PHE:HB2	2.00	0.43
2:C:147:LEU:HD12	2:C:147:LEU:HA	1.90	0.43
1:A:618:ARG:HG2	1:A:619:VAL:N	2.34	0.43
2:D:109:GLN:H	2:D:109:GLN:HG3	1.25	0.42
1:B:520:GLY:HA3	1:B:640:LEU:HD13	2.00	0.42
2:D:90:THR:HG23	2:D:114:THR:HA	2.01	0.42
2:D:24:VAL:HB	2:D:27:PHE:CE1	2.55	0.42
2:C:83:ASN:ND2	3:C:304:HOH:O	2.52	0.42
2:C:93:TYR:O	2:C:110:GLY:HA2	2.19	0.41
2:D:224:GLN:HE21	2:D:226:ASP:HB2	1.83	0.41
1:A:644:LEU:HD23	1:A:644:LEU:HA	1.95	0.41
2:D:39:GLN:HB2	2:D:45:LEU:HD12	2.02	0.41
1:B:482:THR:HA	1:B:483:PRO:HD3	1.88	0.41
2:C:170:TRP:CD2	2:C:208:PHE:HB2	2.56	0.40
2:C:146:LEU:HD23	2:C:146:LEU:HA	1.77	0.40
1:A:502:PRO:HD3	1:A:519:TYR:CE2	2.55	0.40
1:B:503:ILE:HA	1:B:504:PRO:HD3	1.87	0.40
1:B:436:LEU:HD23	1:B:487:VAL:HG13	2.04	0.40
2:D:47:TRP:HZ2	2:D:50:VAL:HG12	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	215/230 (94%)	211 (98%)	4 (2%)	0	100	100
1	B	217/230 (94%)	211 (97%)	6 (3%)	0	100	100
2	C	221/251 (88%)	215 (97%)	6 (3%)	0	100	100
2	D	221/251 (88%)	214 (97%)	7 (3%)	0	100	100
All	All	874/962 (91%)	851 (97%)	23 (3%)	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	197/204 (97%)	189 (96%)	8 (4%)	30	46
1	B	198/204 (97%)	188 (95%)	10 (5%)	24	37
2	C	192/203 (95%)	171 (89%)	21 (11%)	6	9
2	D	192/203 (95%)	169 (88%)	23 (12%)	5	7
All	All	779/814 (96%)	717 (92%)	62 (8%)	12	18

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLU
1	A	497	SER

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Mol	Chain	Res	Type
1	A	542	ARG
1	A	562	SER
1	A	584	GLN
1	A	601	SER
1	A	602	SER
1	A	646	GLN
1	B	468	ILE
1	B	498	ASP
1	B	501	SER
1	B	523	GLN
1	B	526	SER
1	B	537	SER
1	B	549	VAL
1	B	562	SER
1	B	573	ASP
1	B	600	THR
2	C	3	GLN
2	C	17	SER
2	C	19	SER
2	C	25	SER
2	C	51	ILE
2	C	57	THR
2	C	65	SER
2	C	70	SER
2	C	109	GLN
2	C	111	THR
2	C	116	SER
2	C	136	SER
2	C	137	ILE
2	C	149	SER
2	C	191	THR
2	C	195	ASP
2	C	200	SER
2	C	218	LEU
2	C	224	GLN
2	C	231	LEU
2	C	242	LYS
2	D	17	SER
2	D	18	LEU
2	D	19	SER
2	D	25	SER
2	D	31	SER

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Mol	Chain	Res	Type
2	D	40	SER
2	D	56	SER
2	D	66	ARG
2	D	67	LEU
2	D	74	SER
2	D	75	LYS
2	D	95	CYS
2	D	109	GLN
2	D	147	LEU
2	D	152	ASP
2	D	161	SER
2	D	180	LYS
2	D	191	THR
2	D	200	SER
2	D	205	ASP
2	D	207	THR
2	D	241	LEU
2	D	242	LYS

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

Mol	Chain	Res	Type
1	B	522	GLN
1	B	551	ASN
2	C	109	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	217/230 (94%)	-0.23	0 100 100	22, 32, 46, 62	0
1	B	218/230 (94%)	-0.15	0 100 100	24, 35, 51, 64	0
2	C	224/251 (89%)	-0.03	3 (1%) 77 75	27, 40, 62, 83	0
2	D	224/251 (89%)	0.11	7 (3%) 49 45	27, 47, 69, 81	0
All	All	883/962 (91%)	-0.07	10 (1%) 80 79	22, 38, 62, 83	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	145	PHE	3.8
2	D	241	LEU	3.0
2	C	64	ILE	2.8
2	D	83	ASN	2.5
2	D	116	SER	2.5
2	D	43	LYS	2.5
2	D	117	SER	2.3
2	D	13	GLN	2.3
2	C	202[A]	TYR	2.3
2	C	216	GLU	2.2

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 monosaccharides 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.