



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:59 am BST

PDB ID : 5OR7
Title : Atomic structure of the murine norovirus protruding domain and sCD300lf receptor complex
Authors : Kilic, T.; Hansman, G.S.
Deposited on : 2017-08-15
Resolution : 2.05 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	:	2.11
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)	:	2.11

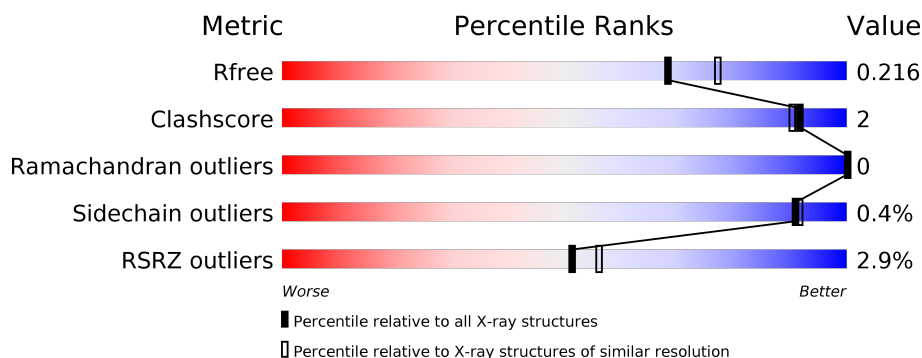
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 on 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	541	<div> <div style="width: 52%;"></div> <div style="width: 45%;"></div> </div>
1	B	541	<div> <div style="width: 52%;"></div> <div style="width: 46%;"></div> </div>
2	C	330	<div> <div style="width: 33%;"></div> <div style="width: 66%;"></div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5832 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2276	1469	368	432	7			
1	B	293	Total	C	N	O	S	0	0	0
			2234	1447	364	416	7			

- Molecule 2 is a protein called CMRF35-like molecule 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	111	Total	C	N	O	S	0	0	0
			857	538	142	170	7			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Na	0	0
			2	2		
3	A	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	200	Total	O	0	0
			200	200		
4	B	175	Total	O	0	0
			175	175		
4	C	84	Total	O	0	0
			84	84		

Chain C: 33% . 66%

ALA	ALA	GLU	ASP	MET
LEU	LEU	GLN	ASN	HIS
THR	THR	GLN	GLY	LEU
LEU	LEU	SER	GLY	SER
ALA	GLY	LEU	GLY	LEU
GLY	GLY	GLU	GLY	VAL
LEU	LEU	GLY	ASP	PRO
GLN	GLY	ASP	SER	PHE
GLU	GLN	LEU	GLY	LEU
GLU	GLU	CYS	GLY	PHE
PRO	THR	TYR	GLY	THR
THR	THR	ALA	GLU	ILE
TYR	TYR	ASP	ASP	THR
GLY	GLY	LEU	GLY	GLY
ASN	ASN	SER	VAL	CYS
THR	THR	LEU	GLY	THR
CYS	CYS	LEU	GLY	CYS
PRO	PRO	PRO	PHE	THR
ILE	ILE	ARG	LEU	ALA
THR	THR	THR	ASP	E1
HIS	HIS	SER	LEU	R23
VAL	VAL	PRO	SER	C36
PRO	PRO	GLY	VAL	I72
ARG	ARG	SER	LEU	THR
THR	THR	SER	LEU	P111
GLY	GLY	TRP	PRO	THR
LEU	LEU	LYS	VAL	MET
GLU	GLU	LYS	ILE	THR
GLU	GLU	SER	SER	PRO
GLU	GLU	SER	ALA	PRO
THR	THR	SER	VAL	ILE
THR	THR	MET	LEU	THR
GLU	GLU	SER	LEU	SER
TYR	TYR	SER	LEU	THR
SER	SER	GLY	LEU	THR
SER	SER	LYS	LEU	ILE
ILE	ILE	ASP	VAL	PHE
ARG	ARG	HIS	ALA	THR
ARG	ARG	GLN	SER	VAL
LEU	LEU	GLU	SER	THR
PRO	PRO	GLU	PHE	THR
ALA	ALA	VAL	ALA	THR
ALA	ALA	GLU	TRP	VAL
MET	MET	TYR	ARG	LYS
PRO	PRO	VAL	MET	GLU
		THR	VAL	THR
		THR	ARG	MET
		MET	ARG	SER
		ALA	ALA	PHE
		PRO	GLN	THR
		PHE	LYS	PRO
		PRO	LYS	THR
		ARG	ALA	LEU
		GLU	ALA	THR
		GLU	GLY	SER
		VAL	PRO	TYR
		SER	PRO	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.11Å 77.46Å 140.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.83 – 2.05 42.82 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.83-2.05) 99.5 (42.82-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.180 , 0.217 0.181 , 0.216	Depositor DCC
R_{free} test set	2620 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5832	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.26	0/2338	0.46	0/3204
1	B	0.26	0/2294	0.47	0/3141
2	C	0.27	0/875	0.50	0/1188
All	All	0.26	0/5507	0.47	0/7533

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	2276	0	2196	10	0
1	B	2234	0	2147	7	0
2	C	857	0	818	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	200	0	0	0	0
4	B	175	0	0	1	0
4	C	84	0	0	0	0
All	All	5832	0	5161	17	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 2.

All (17) 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:338:GLU:OE2	1:B:396:ARG:NH1	2.22	0.72
2:C:23:ARG:HG2	2:C:72:ILE:HG12	1.79	0.65
1:A:267:GLY:HA2	1:A:458:ILE:HD11	1.87	0.55
1:A:490:LYS:HG3	1:A:527:LEU:HD21	1.89	0.55
1:B:270:HIS:CE1	1:B:276:LEU:HD11	2.44	0.52
1:A:270:HIS:CE1	1:A:276:LEU:HD11	2.46	0.50
1:A:340:GLN:HG2	1:A:350:LEU:HD22	1.95	0.48
1:B:263:GLN:NE2	4:B:704:HOH:O	2.36	0.48
1:B:399:TYR:CE1	1:B:440:ASP:HB3	2.51	0.46
1:B:440:ASP:OD1	1:B:440:ASP:N	2.49	0.46
1:A:399:TYR:CE2	1:A:440:ASP:HB3	2.52	0.45
1:A:230:VAL:HG22	1:A:466:PHE:HB3	1.98	0.45
1:B:230:VAL:HG22	1:B:466:PHE:HB3	1.99	0.44
1:A:267:GLY:HA2	1:A:458:ILE:CD1	2.48	0.43
1:A:355:PHE:CE1	1:A:378:LEU:HD23	2.54	0.42
1:B:490:LYS:HG3	1:B:527:LEU:HD21	2.03	0.41
1:A:269:VAL:O	1:A:495:GLY:HA3	2.21	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	291/541 (54%)	282 (97%)	9 (3%)	0	100	100
1	B	283/541 (52%)	276 (98%)	7 (2%)	0	100	100
2	C	109/330 (33%)	107 (98%)	2 (2%)	0	100	100
All	All	683/1412 (48%)	665 (97%)	18 (3%)	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	242/449 (54%)	241 (100%)	1 (0%)	91	91
1	B	232/449 (52%)	232 (100%)	0	100	100
2	C	95/283 (34%)	94 (99%)	1 (1%)	73	73
All	All	569/1181 (48%)	567 (100%)	2 (0%)	91	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	GLU
2	C	36	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	297/541 (54%)	-0.01	6 (2%) 65 69	18, 28, 52, 82	0
1	B	293/541 (54%)	-0.03	14 (4%) 30 33	17, 27, 52, 87	0
2	C	111/330 (33%)	-0.28	0 100 100	19, 26, 37, 57	0
All	All	701/1412 (49%)	-0.06	20 (2%) 51 56	17, 27, 51, 87	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	ALA	5.7
1	B	301	THR	4.7
1	A	345	LYS	4.0
1	B	297	PHE	3.7
1	A	445	ALA	3.1
1	A	483	GLY	3.1
1	B	360	GLY	3.1
1	B	299	SER	3.1
1	B	296	GLU	3.0
1	B	298	GLN	2.9
1	B	445	ALA	2.9
1	B	383	SER	2.6
1	A	481	LEU	2.6
1	B	386	LEU	2.5
1	B	361	PRO	2.3
1	B	378	LEU	2.3
1	B	399	TYR	2.2
1	A	344	THR	2.2
1	A	228	ARG	2.1
1	B	350	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	A	601	1/1	0.93	0.26	47,47,47,47	0
3	NA	B	601	1/1	0.96	0.16	44,44,44,44	0
3	NA	C	401	1/1	0.97	0.07	26,26,26,26	0
3	NA	A	600	1/1	0.98	0.10	27,27,27,27	0
3	NA	C	402	1/1	0.98	0.40	39,39,39,39	0
3	NA	B	600	1/1	0.99	0.06	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.