



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:17 AM GMT

PDB ID : 2GHW
Title : Crystal structure of SARS spike protein receptor binding domain in complex with a neutralizing antibody, 80R
Authors : Hwang, W.C.; Lin, Y.; Santelli, E.; Sui, J.; Jaroszewski, L.; Stec, B.; Farzan, M.; Marasco, W.A.; Liddington, R.C.
Deposited on : 2006-03-27
Resolution : 2.30 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
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

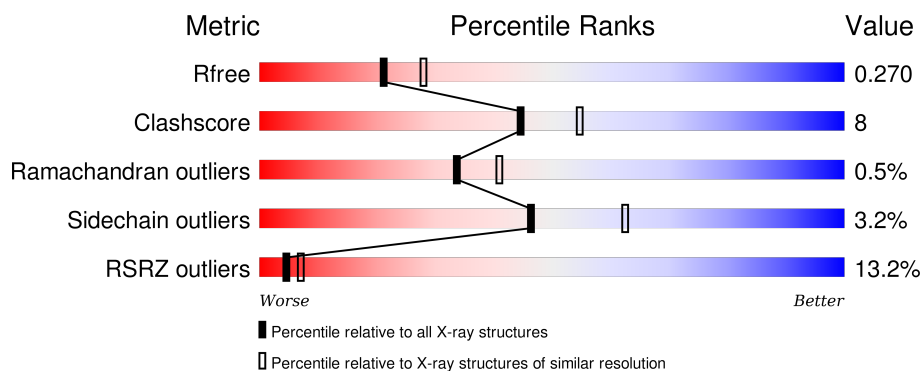
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	203	<div> <div>18%</div> <div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>
1	C	203	<div> <div>13%</div> <div> <div>78%</div> <div>13%</div> <div>7%</div> </div> </div>
2	B	247	<div> <div>11%</div> <div> <div>76%</div> <div>16%</div> <div>6%</div> </div> </div>
2	D	247	<div> <div>9%</div> <div> <div>78%</div> <div>14%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	517	-	-	X	-
3	CL	A	88	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7089 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 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1528	989	248	283	8			
1	C	188	Total	C	N	O	S	0	0	0
			1512	978	246	280	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	314	MET	-	CLONING ARTIFACT	UNP P59594
C	315	ALA	-	CLONING ARTIFACT	UNP P59594
C	316	ASP	-	CLONING ARTIFACT	UNP P59594
C	511	SER	-	CLONING ARTIFACT	UNP P59594
C	512	GLY	-	CLONING ARTIFACT	UNP P59594
C	513	LEU	-	CLONING ARTIFACT	UNP P59594
C	514	VAL	-	CLONING ARTIFACT	UNP P59594
C	515	PRO	-	CLONING ARTIFACT	UNP P59594
C	516	ARG	-	CLONING ARTIFACT	UNP P59594
A	314	MET	-	CLONING ARTIFACT	UNP P59594
A	315	ALA	-	CLONING ARTIFACT	UNP P59594
A	316	ASP	-	CLONING ARTIFACT	UNP P59594
A	511	SER	-	CLONING ARTIFACT	UNP P59594
A	512	GLY	-	CLONING ARTIFACT	UNP P59594
A	513	LEU	-	CLONING ARTIFACT	UNP P59594
A	514	VAL	-	CLONING ARTIFACT	UNP P59594
A	515	PRO	-	CLONING ARTIFACT	UNP P59594
A	516	ARG	-	CLONING ARTIFACT	UNP P59594

- Molecule 2 is a protein called anti-sars scFv antibody, 80R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	232	Total	C	N	O	S	0	0	0
			1785	1118	312	349	6			

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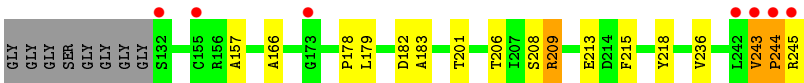
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	231	Total	C	N	O	S	0	0	0
			1789	1120	314	349	6			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	118	Total	O	0	0
			118	118		
4	C	115	Total	O	0	0
			115	115		
4	D	129	Total	O	0	0
			129	129		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.45Å 175.90Å 67.56Å 90.00° 96.55° 90.00°	Depositor
Resolution (Å)	45.55 – 2.30 47.14 – 2.19	Depositor EDS
% Data completeness (in resolution range)	93.8 (45.55-2.30) 91.5 (47.14-2.19)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.295 0.263 , 0.270	Depositor DCC
R_{free} test set	2300 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	1.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 51874 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7089	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 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:
CL

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	0.47	0/1576	0.60	0/2152
1	C	0.47	0/1559	0.61	0/2127
2	B	0.42	0/1827	0.65	1/2481 (0.0%)
2	D	0.44	0/1831	0.61	0/2485
All	All	0.45	0/6793	0.62	1/9245 (0.0%)

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	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	156	ARG	NE-CZ-NH1	7.00	123.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	102	TYR	Peptide
2	D	102	TYR	Peptide

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	1528	0	1455	26	0
1	C	1512	0	1439	20	0
2	B	1785	0	1722	27	0
2	D	1789	0	1729	29	0
3	A	4	0	0	5	0
3	C	1	0	0	1	0
4	A	108	0	0	4	0
4	B	118	0	0	2	0
4	C	115	0	0	0	0
4	D	129	0	0	1	0
All	All	7089	0	6345	102	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 8.

The worst 5 of 102 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)
2:B:39:GLN:HE22	2:B:170:GLN:HE22	1.31	0.77
1:A:472:LEU:HD13	2:B:206:THR:HG21	1.67	0.75
3:A:88:CL:CL	4:B:411:HOH:O	2.42	0.75
2:B:40:ALA:HB3	2:B:43:LYS:HG2	1.71	0.72
1:A:322:LEU:HD12	1:A:349:VAL:CG2	2.20	0.72

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	189/203 (93%)	178 (94%)	11 (6%)	0	100	100
1	C	186/203 (92%)	171 (92%)	15 (8%)	0	100	100
2	B	228/247 (92%)	211 (92%)	16 (7%)	1 (0%)	39	48
2	D	227/247 (92%)	214 (94%)	10 (4%)	3 (1%)	15	15
All	All	830/900 (92%)	774 (93%)	52 (6%)	4 (0%)	34	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	209	ARG
2	D	243	VAL
2	B	118	GLY
2	D	244	PRO

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	167/177 (94%)	164 (98%)	3 (2%)	66	82
1	C	166/177 (94%)	161 (97%)	5 (3%)	48	65
2	B	192/196 (98%)	183 (95%)	9 (5%)	32	43
2	D	193/196 (98%)	187 (97%)	6 (3%)	47	64
All	All	718/746 (96%)	695 (97%)	23 (3%)	46	62

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	213	GLU
1	C	319	ILE
2	D	213	GLU
2	B	242	LEU
1	C	321	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	174	GLN
1	C	321	ASN
2	D	35	HIS
2	B	82	GLN
2	D	57	ASN

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 5 ligands modelled in this entry, 5 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 [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	191/203 (94%)	1.37	36 (18%) 2 2	15, 21, 32, 42	1 (0%)
1	C	188/203 (92%)	1.23	27 (14%) 3 5	15, 21, 30, 41	0
2	B	232/247 (93%)	0.95	26 (11%) 7 10	14, 20, 26, 38	2 (0%)
2	D	231/247 (93%)	1.00	22 (9%) 10 15	15, 20, 25, 44	2 (0%)
All	All	842/900 (93%)	1.12	111 (13%) 4 7	14, 20, 29, 44	5 (0%)

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	244	PRO	10.8
1	A	507	PRO	9.1
1	A	506	ALA	8.7
1	A	319	ILE	8.5
2	B	244	PRO	7.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	A	88	1/1	0.95	0.24	3.46	3,3,3,3	0
3	CL	C	20	1/1	0.98	0.15	0.17	11,11,11,11	0
3	CL	A	246	1/1	0.93	0.29	-	14,14,14,14	0
3	CL	A	142	1/1	0.96	0.21	-	8,8,8,8	0
3	CL	A	517	1/1	0.95	0.27	-	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.