W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Preliminary Full wwPDB X-ray Structure Validation Report ⓘ

Aug 12, 2022 – 06:43 PM JST

Deposition ID : D_1300031561

<div style="border:2px solid red">

This wwPDB validation report is NOT for manuscript review

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This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

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:

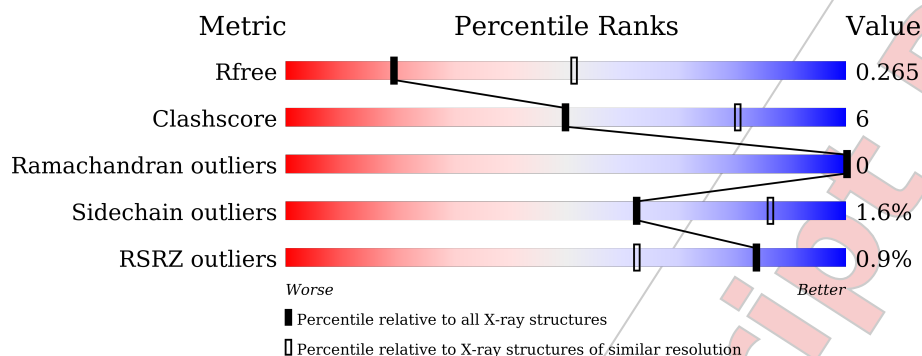|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 3.00 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		0.9%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	112	88% 12% •
1	B	112	% 79% 21%
2	D	107	2% 87% 13%
3	C	105	% 86% 14%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3363 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	0	0
			875	552	151	168	4			
1	B	112	Total	C	N	O	S	0	0	0
			875	552	151	168	4			

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	107	Total	C	N	O	S	0	0	0
			816	510	144	155	7			

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	S	0	0	0
			797	498	139	153	7			

3 Residue-property plots ⓘ

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.
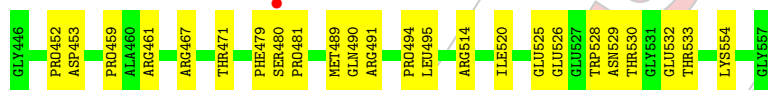
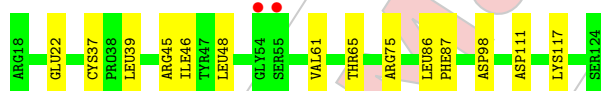- Molecule 1:

Chain A:

88% 12%

GLY446 PRO452 THR471 PHE479 PHE485 ILE520 VAL523 ASN529 THR530 GLY531 GLU532 ALA539 VAL552 ASP553 LYS554 SER555 THR556 GLY557

- Molecule 1:

Chain B:

%

79% 21%

GLY446 PRO452 ASP453 PRO459 ALA460 ARG461 ARG467 THR471 PHE479 SER480 PRO481 MET489 GLN490 ARG491 PRO494 LEU495 ARG514 ILE520 GLU525 GLU526 GLU527 TRP528 ASN529 THR530 GLY531 GLU532 THR533 LYS554 GLY557

- Molecule 2:

Chain D:

2%

87% 13%

ARG18 GLU22 CYS37 PRO38 LEU39 ARG45 ILE46 TYR47 LEU48 GLY54 SER55 VAL61 THR65 ARG75 LEU86 PHE87 ASP98 ASP111 LYS117 SER124

- Molecule 3:

Chain C:

%

86% 14%

LEU20 PRO21 GLU26 VAL33 MET42 TYR47 THR57 LYS69 ALA70 GLU71 LEU94 THR95 GLU96 THR110 ASP111 ARG112 GLY113 GLN116 HIS123 SER124

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	85.72Å 85.72Å 60.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.08 – 3.00 28.08 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.5 (28.08-3.00) 95.5 (28.08-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.230 , 0.269 0.225 , 0.265	Depositor DCC
R_{free} test set	491 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 22.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l 0.048 for h,-h-k,-l 0.032 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3363	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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	0.51	0/899	0.63	0/1232
1	B	0.33	0/899	0.56	0/1232
2	D	0.38	0/827	0.57	0/1115
3	C	0.34	0/808	0.57	0/1090
All	All	0.40	0/3433	0.58	0/4669

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 (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	875	0	848	7	0
1	B	875	0	848	16	0
2	D	816	0	835	8	0
3	C	797	0	811	9	0
All	All	3363	0	3342	39	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 6.

All (39) 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)
3:C:26:GLU:OE1	3:C:123:HIS:NE2	1.69	1.24
3:C:26:GLU:OE1	3:C:123:HIS:CD2	2.32	0.82
3:C:47:TYR:OH	3:C:113:GLY:O	2.01	0.78
2:D:75:ARG:NH2	2:D:98:ASP:OD2	2.26	0.69
1:B:529:ASN:HA	1:B:554:LYS:HE2	1.84	0.59
1:B:525:GLU:OE2	1:B:529:ASN:ND2	2.35	0.58
1:B:490:GLN:HB3	1:B:495:LEU:HD21	1.87	0.57
1:B:467:ARG:NH1	2:D:111:ASP:HB2	2.20	0.56
3:C:21:PRO:HB2	3:C:116:GLN:HG3	1.87	0.56
1:A:452:PRO:HB3	1:A:479:PHE:HB3	1.90	0.54
1:B:471:THR:HG23	1:B:520:ILE:HG23	1.90	0.52
1:B:491:ARG:HH12	1:B:533:THR:HB	1.76	0.51
2:D:22:GLU:HG3	2:D:117:LYS:HE2	1.94	0.50
3:C:96:GLU:OE2	3:C:124:SER:OG	2.30	0.50
1:B:452:PRO:HG3	1:B:479:PHE:HB3	1.95	0.48
1:B:467:ARG:HD3	1:B:525:GLU:OE1	2.13	0.48
3:C:33:VAL:HG13	3:C:94:LEU:HD11	1.96	0.48
1:B:480:SER:HB3	1:B:481:PRO:HD3	1.96	0.48
2:D:39:LEU:HD13	2:D:87:PHE:HB3	1.96	0.48
1:A:529:ASN:HA	1:A:554:LYS:HE2	1.95	0.48
2:D:48:LEU:O	2:D:61:VAL:HG22	2.14	0.48
3:C:57:THR:OG1	3:C:111:ASP:OD2	2.23	0.47
1:B:491:ARG:HA	1:B:491:ARG:HD3	1.63	0.47
1:A:554:LYS:H	1:A:554:LYS:HG3	1.43	0.46
1:A:485:PHE:HB3	1:A:539:ALA:HB3	1.97	0.45
1:B:461:ARG:HG3	1:B:461:ARG:HH11	1.82	0.45
2:D:45:ARG:HG3	2:D:65:THR:OG1	2.16	0.45
1:A:471:THR:HG23	1:A:520:ILE:HG23	1.98	0.45
1:B:489:MET:HG2	1:B:494:PRO:HA	2.00	0.44
1:B:491:ARG:NH2	1:B:532:GLU:HA	2.32	0.43
3:C:47:TYR:CE1	3:C:110:THR:HG23	2.54	0.43
1:B:526:GLU:O	1:B:530:THR:HG23	2.18	0.43
1:B:459:PRO:HD2	1:B:528:TRP:CZ2	2.54	0.43
1:A:531:GLY:HA2	1:A:554:LYS:HD2	2.01	0.41
3:C:69:LYS:HG2	3:C:71:GLU:OE1	2.20	0.41
1:B:461:ARG:HG3	1:B:461:ARG:NH1	2.35	0.41
2:D:37:CYS:O	2:D:86:LEU:HD12	2.21	0.41
2:D:46:ILE:HG23	2:D:87:PHE:CZ	2.56	0.41
1:A:530:THR:OG1	1:A:532:GLU:HG2	2.21	0.40

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	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
1	B	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
2	D	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
3	C	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
All	All	428/436 (98%)	416 (97%)	12 (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	97/97 (100%)	93 (96%)	4 (4%)	30	67
1	B	97/97 (100%)	95 (98%)	2 (2%)	53	82
2	D	92/92 (100%)	92 (100%)	0	100	100
3	C	90/90 (100%)	90 (100%)	0	100	100
All	All	376/376 (100%)	370 (98%)	6 (2%)	62	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	523	VAL
1	A	552	VAL

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Mol	Chain	Res	Type
1	A	554	LYS
1	A	555	SER
1	B	453	ASP
1	B	514	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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(Å²)	Q<0.9
1	A	112/112 (100%)	-0.35	0	100	100	28, 42, 73, 87	0
1	B	112/112 (100%)	-0.22	1 (0%)	84	63	31, 52, 74, 85	0
2	D	107/107 (100%)	-0.34	2 (1%)	66	37	25, 41, 77, 93	0
3	C	105/105 (100%)	-0.24	1 (0%)	82	59	36, 46, 74, 98	0
All	All	436/436 (100%)	-0.29	4 (0%)	84	63	25, 45, 74, 98	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	55	SER	3.2
3	C	42	MET	2.8
2	D	54	GLY	2.7
1	B	480	SER	2.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

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6.5 Other polymers ⓘ

There are no such residues in this entry.