Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 10:23 AM EDT

PDB ID	:	2ARR
Title	:	Human plasminogen activator inhibitor-2.[loop (66-98) deletion mutant] complexed with peptide n-acetyl-teaaagmggvmtgr-oh
Authors	:	Di Giusto, D.A.; Sutherland, A.P.; Jankova, L.; Harrop, S.J.; Curmi, P.M.; King, G.C.
Deposited on	:	2005-08-21
Resolution	:	1.55 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 (i) 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 (i)) were used in the production of this report:

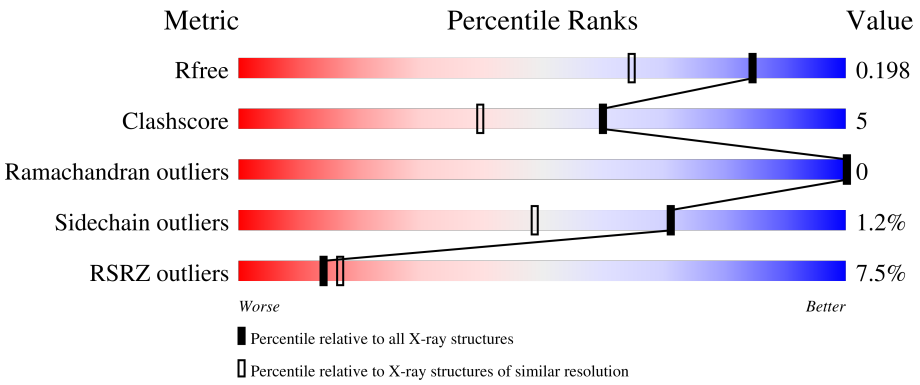
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	382	7%, 84%, 9%, 6%
2	P	15	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3380 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 Plasminogen activator inhibitor-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2962	1887	493	561	21	0	14	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	SER	LYS	conflict	UNP P05120
A	?	-	ASN	deletion	UNP P05120
A	?	-	ALA	deletion	UNP P05120
A	?	-	VAL	deletion	UNP P05120
A	?	-	THR	deletion	UNP P05120
A	?	-	PRO	deletion	UNP P05120
A	?	-	MET	deletion	UNP P05120
A	?	-	THR	deletion	UNP P05120
A	?	-	PRO	deletion	UNP P05120
A	?	-	GLU	deletion	UNP P05120
A	?	-	ASN	deletion	UNP P05120
A	?	-	PHE	deletion	UNP P05120
A	?	-	THR	deletion	UNP P05120
A	?	-	SER	deletion	UNP P05120
A	?	-	CYS	deletion	UNP P05120
A	?	-	GLY	deletion	UNP P05120
A	?	-	PHE	deletion	UNP P05120
A	?	-	MET	deletion	UNP P05120
A	?	-	GLN	deletion	UNP P05120
A	?	-	GLN	deletion	UNP P05120
A	?	-	ILE	deletion	UNP P05120
A	?	-	GLN	deletion	UNP P05120
A	?	-	LYS	deletion	UNP P05120
A	?	-	GLY	deletion	UNP P05120
A	?	-	SER	deletion	UNP P05120
A	?	-	TYR	deletion	UNP P05120
A	?	-	PRO	deletion	UNP P05120

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P05120
A	?	-	ALA	deletion	UNP P05120
A	?	-	ILE	deletion	UNP P05120
A	?	-	LEU	deletion	UNP P05120
A	?	-	GLN	deletion	UNP P05120
A	?	-	ALA	deletion	UNP P05120
A	?	-	GLN	deletion	UNP P05120
A	220	PHE	TYR	conflict	UNP P05120

- Molecule 2 is a protein called 14-mer from Plasminogen activator inhibitor-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	P	15	92	53	17	20	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	351	MET	THR	engineered mutation	UNP P05120

- Molecule 3 is water.

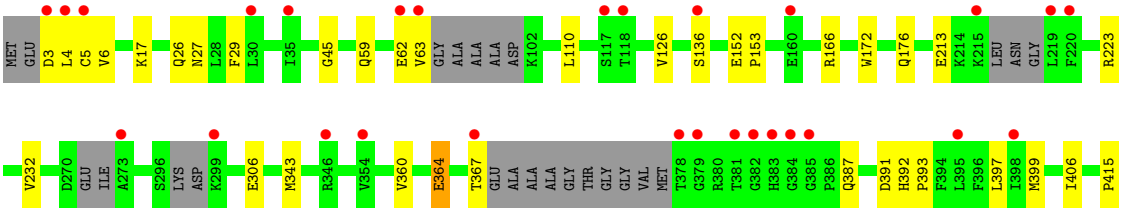
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	322	322	322	0	0
			Total	O		
3	P	4	4	4	0	0

3 Residue-property plots (i)

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.

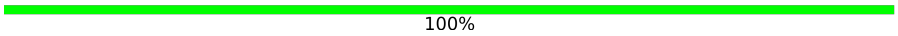
• Molecule 1: Plasminogen activator inhibitor-2

Chain A:



• Molecule 2: 14-mer from Plasminogen activator inhibitor-2

Chain P:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	91.95Å 103.80Å 41.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.70 – 1.55 30.77 – 1.55	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.70-1.55) 97.3 (30.77-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.220 0.200 , 0.198	Depositor DCC
R_{free} test set	2851 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3380	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.85	0/3021	0.86	2/4064 (0.0%)
2	P	0.85	0/89	0.81	0/116
All	All	0.85	0/3110	0.86	2/4180 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	391	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	166	ARG	NE-CZ-NH1	5.26	122.93	120.30

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	2962	0	2905	28	0
2	P	92	0	90	0	0
3	A	322	0	0	6	0
3	P	4	0	0	0	0
All	All	3380	0	2995	28	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 (28) 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:397:LEU:HD13	1:A:399[B]:MET:SD	2.04	0.97
1:A:397:LEU:CD1	1:A:399[B]:MET:SD	2.64	0.85
1:A:399[B]:MET:SD	1:A:406:ILE:HG12	2.34	0.68
1:A:3:ASP:O	1:A:6:VAL:HG23	1.96	0.65
1:A:397:LEU:HD12	1:A:399[B]:MET:HG2	1.80	0.64
1:A:397:LEU:CD1	1:A:399[B]:MET:HG2	2.28	0.64
1:A:26:GLN:HE21	1:A:27:ASN:H	1.47	0.62
1:A:397:LEU:CD1	1:A:399[B]:MET:CG	2.80	0.60
1:A:17:LYS:HG3	3:A:656:HOH:O	2.02	0.59
1:A:306:GLU:CD	1:A:387:GLN:HE22	2.10	0.54
1:A:59:GLN:OE1	1:A:62:GLU:HG3	2.08	0.53
1:A:213:GLU:HG3	3:A:613:HOH:O	2.10	0.52
1:A:232:VAL:HG12	1:A:415:PRO:HB3	1.91	0.52
1:A:4:LEU:HD12	3:A:710:HOH:O	2.10	0.51
1:A:152:GLU:N	1:A:153:PRO:HD3	2.29	0.48
1:A:172:TRP:O	1:A:176:GLN:HG2	2.13	0.48
1:A:3:ASP:HB3	1:A:6:VAL:CG2	2.44	0.47
1:A:392:HIS:HE1	3:A:417:HOH:O	1.97	0.46
1:A:5[B]:CYS:SG	1:A:110:LEU:HD22	2.56	0.46
1:A:45:GLY:HA3	1:A:343:MET:HG3	1.99	0.45
1:A:232:VAL:CG1	1:A:415:PRO:HB3	2.48	0.44
1:A:29:PHE:CZ	1:A:360:VAL:HB	2.52	0.43
1:A:126:VAL:HG22	3:A:646:HOH:O	2.19	0.43
1:A:364:GLU:CD	1:A:364:GLU:H	2.22	0.43
1:A:223[B]:ARG:O	1:A:393:PRO:HD3	2.19	0.42
1:A:26:GLN:HG3	1:A:27:ASN:N	2.34	0.42
1:A:392:HIS:HD2	3:A:527:HOH:O	2.03	0.41
1:A:232:VAL:HG11	1:A:415:PRO:CG	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	360/382 (94%)	352 (98%)	8 (2%)	0	100	100
2	P	13/15 (87%)	13 (100%)	0	0	100	100
All	All	373/397 (94%)	365 (98%)	8 (2%)	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	330/329 (100%)	326 (99%)	4 (1%)	71	49
2	P	7/7 (100%)	7 (100%)	0	100	100
All	All	337/336 (100%)	333 (99%)	4 (1%)	71	49

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	VAL
1	A	136	SER
1	A	364	GLU
1	A	367	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	387	GLN
1	A	392	HIS
1	A	404	ASN

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 monosaccharides 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 (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	358/382 (93%)	0.57	28 (7%) 13 15	15, 24, 37, 51	0
2	P	14/15 (93%)	0.57	0 100 100	17, 20, 28, 31	0
All	All	372/397 (93%)	0.57	28 (7%) 14 17	15, 23, 36, 51	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	THR	8.1
1	A	63	VAL	7.9
1	A	378	THR	6.8
1	A	4	LEU	6.3
1	A	273	ALA	6.0
1	A	385	GLY	5.5
1	A	219	LEU	5.0
1	A	136	SER	4.8
1	A	383	HIS	4.0
1	A	382	GLY	4.0
1	A	3	ASP	3.9
1	A	346	ARG	3.9
1	A	384	GLY	3.6
1	A	379	GLY	3.6
1	A	220	PHE	3.5
1	A	299	LYS	3.0
1	A	118	THR	2.9
1	A	62	GLU	2.7
1	A	395	LEU	2.6
1	A	117	SER	2.5
1	A	35	ILE	2.5
1	A	30[A]	LEU	2.5
1	A	5[A]	CYS	2.4
1	A	215	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	398	ILE	2.4
1	A	354	VAL	2.3
1	A	367	THR	2.2
1	A	160	GLU	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 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.