

Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 02:06 PM JST

PDB ID	:	8GZO
Title	:	Crystal structure of collagen heterotrimer with K, D, E, R residuesC
Authors	:	Fan, S.
Deposited on		
Resolution	:	1.23 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 (1)) were used in the production of this report:

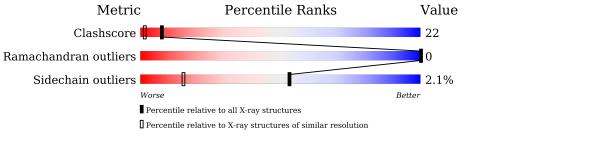
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.23 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	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	32	72%	22%	6%
2	В	32	84%	12	2% •
3	С	32	69%	25%	• •



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 888 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 collagen-like peptide.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
1	А	32	Total 220	C 135	N 39	O 46	0	1	0

• Molecule 2 is a protein called collagen-like peptide.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
2	В	32	Total 211	C 119	N 36	O 56	0	1	0

• Molecule 3 is a protein called collagen-like peptide.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
3	С	31	Total 214	C 134	N 39	0 41	0	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	79	Total O 79 79	0	0
4	В	82	TotalO8282	0	0
4	С	82	TotalO8282	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. 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. 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.

Note EDS was not executed.

• Molecule 1: collagen-like peptide

Chain A:	72%	22% 6	6%
Y1 K4 F9 F13 F13 F13 F21 F22 G20 G20 G20 G23 G23 G23 G23 G23 G23 G23 G23 G23 G23	6 33 31 - 52 93 31 - 5		
• Molecule 2: collag	gen-like peptide		
Chain B:	84%	12%	·
11 P7 P10 P10 P13 P31 P31 C32			
• Molecule 3: collag	gen-like peptide		
Chain C:	69%	25% •	·
Y1 Y1 Y1 Y1 Y1 Y1 Y1 Y1 Y1 Y1	22 1-23 0 CT A		



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	61.30Å 42.45Å 28.93Å	Depositor
a, b, c, α , β , γ	90.00° 105.46° 90.00°	Depositor
Resolution (Å)	18.02 - 1.23	Depositor
% Data completeness	89.9 (18.02-1.23)	Depositor
(in resolution range)	05.5 (10.02 1.25)	Depositor
R_{merge}	0.04	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.174 , 0.190	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	888	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP



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: HYP

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	А	0.61	0/189	0.77	0/242	
2	В	0.57	0/169	0.89	0/219	
3	С	0.61	0/169	0.90	0/210	
All	All	0.60	0/527	0.85	0/671	

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	А	220	0	210	17	0
2	В	211	0	159	2	0
3	С	214	0	220	9	0
4	А	79	0	0	21	3
4	В	82	0	0	1	2
4	С	82	0	0	4	2
All	All	888	0	589	27	5

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 22.



A. 1	A.L. D.	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:A:103:HOH:O	3:C:22:HYP:HA	1.35	1.26
3:C:25:HYP:HD23	4:C:127:HOH:O	1.32	1.24
1:A:21:ASP:HB2	4:A:109:HOH:O	1.37	1.22
3:C:24:LYS:HA	4:C:127:HOH:O	1.51	1.10
1:A:31:LYS:HD2	4:A:161:HOH:O	1.52	1.08
1:A:31:LYS:CD	4:A:161:HOH:O	2.04	1.05
1:A:31:LYS:HE2	4:A:161:HOH:O	1.62	0.97
1:A:24:ASP:N	4:A:103:HOH:O	2.11	0.82
1:A:24:ASP:O	4:A:101:HOH:O	1.98	0.80
1:A:31:LYS:CE	4:A:161:HOH:O	2.15	0.76
1:A:21:ASP:OD1	4:A:102:HOH:O	2.07	0.73
1:A:21:ASP:CB	4:A:109:HOH:O	2.14	0.68
4:A:101:HOH:O	3:C:23:GLY:N	2.17	0.68
4:A:101:HOH:O	3:C:23:GLY:HA3	1.93	0.67
2:B:13:HYP:O	4:B:101:HOH:O	2.13	0.67
4:A:111:HOH:O	3:C:13:LYS:HE3	1.94	0.67
1:A:31:LYS:O	4:A:104:HOH:O	2.14	0.64
1:A:24:ASP:O	4:A:103:HOH:O	2.15	0.63
1:A:4:LYS:NZ	4:A:107:HOH:O	2.32	0.61
4:A:101:HOH:O	3:C:23:GLY:CA	2.44	0.61
1:A:31:LYS:HD2	4:A:156:HOH:O	2.15	0.46
1:A:21:ASP:N	4:A:109:HOH:O	2.49	0.46
1:A:25:HYP:HA	4:A:101:HOH:O	2.16	0.45
2:B:22:ASP:OD1	3:C:23:GLY:HA2	2.17	0.45
1:A:9:PRO:HG2	4:C:144:HOH:O	2.15	0.45
1:A:24:ASP:CA	4:A:103:HOH:O	2.63	0.43
3:C:15:LYS:NZ	4:C:101:HOH:O	2.20	0.41

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:173:HOH:O	4:C:175:HOH:O[3_455]	1.81	0.39
4:A:153:HOH:O	4:A:171:HOH:O[2_555]	1.92	0.28
4:A:176:HOH:O	4:B:181:HOH:O[2_556]	1.92	0.28
4:A:161:HOH:O	4:A:161:HOH:O[2_756]	1.99	0.21
4:C:105:HOH:O	4:C:111:HOH:O[3_455]	2.03	0.17



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	Perce	ntiles
1	А	26/32~(81%)	26 (100%)	0	0	100	100
2	В	25/32~(78%)	25 (100%)	0	0	100	100
3	С	24/32~(75%)	24 (100%)	0	0	100	100
All	All	75/96~(78%)	75 (100%)	0	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percent	iles
1	А	17/17~(100%)	16 (94%)	1 (6%)	19	1
2	В	15/16~(94%)	15 (100%)	0	100 1	L00
3	С	15/15~(100%)	15 (100%)	0	100 1	L00
All	All	47/48~(98%)	46 (98%)	1 (2%)	53 1	15

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	21	ASP

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



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	B	ond leng	<i>,</i>	В	ond ang	gles
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	HYP	А	19	1	6,8,9	1.08	0	$5,\!10,\!12$	2.04	1 (20%)
1	HYP	А	13	1	6,8,9	1.16	1 (16%)	5,10,12	1.56	1 (20%)
2	HYP	В	7	2	6,8,9	1.16	0	5,10,12	1.44	1 (20%)
2	HYP	В	13	2	6,8,9	1.22	1 (16%)	5,10,12	1.72	1 (20%)
3	HYP	С	16	3	6,8,9	0.82	0	5,10,12	1.80	2 (40%)
3	HYP	С	22	3	6,8,9	1.09	0	5,10,12	1.76	1 (20%)
3	HYP	С	25	3	6,8,9	0.97	0	$5,\!10,\!12$	1.29	0
3	HYP	С	28	3	6,8,9	1.11	1 (16%)	5,10,12	1.65	1 (20%)
3	HYP	С	4	3	6,8,9	1.35	1 (16%)	5,10,12	2.68	3 (60%)
2	HYP	В	31	2	6,8,9	0.99	0	5,10,12	1.87	1 (20%)
3	HYP	С	31	3	3,3,9	0.61	0	0,2,12	-	-
2	HYP	В	19	2	6,8,9	1.02	0	5,10,12	1.53	0
2	HYP	В	10	2	6,8,9	1.03	0	5,10,12	1.16	1 (20%)
1	HYP	А	22	1	6,8,9	0.97	0	5,10,12	1.46	1 (20%)
1	HYP	А	25	1	6,8,9	1.10	1 (16%)	5,10,12	1.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	А	19	1	-	0/0/11/13	0/1/1/1
1	HYP	А	13	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	В	7	2	-	0/0/11/13	0/1/1/1
2	HYP	В	13	2	-	0/0/11/13	0/1/1/1
3	HYP	С	16	3	-	0/0/11/13	0/1/1/1
3	HYP	С	22	3	-	0/0/11/13	0/1/1/1
3	HYP	С	25	3	-	0/0/11/13	0/1/1/1
3	HYP	С	28	3	-	0/0/11/13	0/1/1/1
3	HYP	С	4	3	-	0/0/11/13	0/1/1/1
2	HYP	В	31	2	-	0/0/11/13	0/1/1/1
3	HYP	С	31	3	-	0/0/1/13	-
2	HYP	В	19	2	-	0/0/11/13	0/1/1/1
2	HYP	В	10	2	-	0/0/11/13	0/1/1/1
1	HYP	А	22	1	-	0/0/11/13	0/1/1/1
1	HYP	А	25	1	-	0/0/11/13	0/1/1/1

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All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	25	HYP	OD1-CG	-2.21	1.36	1.43
3	С	4	HYP	CB-CG	-2.06	1.48	1.52
2	В	13	HYP	OD1-CG	-2.03	1.37	1.43
3	С	28	HYP	OD1-CG	-2.03	1.37	1.43
1	А	13	HYP	CB-CG	-2.02	1.48	1.52

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	С	4	HYP	CG-CB-CA	-3.89	99.05	103.96
1	А	19	HYP	CB-CG-CD	-3.79	98.62	103.27
3	С	4	HYP	CB-CG-CD	-3.60	98.85	103.27
2	В	13	HYP	CB-CG-CD	-3.17	99.38	103.27
3	С	22	HYP	CB-CG-CD	-3.09	99.48	103.27
2	В	31	HYP	CB-CG-CD	-2.91	99.70	103.27
2	В	7	HYP	CB-CG-CD	-2.61	100.07	103.27
3	С	16	HYP	CB-CG-CD	-2.45	100.27	103.27
3	С	28	HYP	CB-CG-CD	-2.40	100.33	103.27
1	А	13	HYP	OD1-CG-CD	-2.31	105.31	110.35
1	А	22	HYP	CB-CG-CD	-2.30	100.45	103.27
2	В	10	HYP	CB-CG-CD	-2.22	100.54	103.27
3	С	4	HYP	O-C-CA	-2.16	119.11	124.78
3	С	16	HYP	CG-CB-CA	-2.11	101.30	103.96

All (14) bond angle outliers are listed below:

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	13	HYP	1	0
3	С	22	HYP	1	0
3	С	25	HYP	1	0
1	А	25	HYP	1	0

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

