

wwPDB X-ray Structure Validation Summary Report (i)

Sep 27, 2022 - 11:00 am BST

PDB ID	:	7ZMV
Title	:	Crystal structure of human RECQL5 helicase APO form in complex with
		engineered nanobody (Gluebody) G5-006
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Deposited on	:	2022-04-19
Resolution	:	2.00 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 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.31.2
Xtriage (Phenix) EDS Percentile statistics Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	: : : :	 1.13 FAILED 20191225.v01 (using entries in the PDB archive December 25th 2019 Engh & Huber (2001) Parkinson et al. (1996) 2.31.2

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 2.00 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.



Motria	Whole archive	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
Clashscore	141614	$9178 \ (2.00-2.00)$		
Ramachandran outliers	138981	9054 (2.00-2.00)		
Sidechain outliers	138945	9053 (2.00-2.00)		

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain		
1	А	445	84%	14%	••
1	В	445	86%	12%	·
1	С	445	87%	11%	·
1	D	445	86%	13%	·
2	Е	127	83%	14%	·
2	F	127	82%	16%	·
2	G	127	81%	17%	·
2	K	127	83%	14%	·



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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18647 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	Λ	440	Total	С	Ν	0	\mathbf{S}	0	F	0	
	A	440	3455	2182	623	627	23	0	5	0	
1	В	440	Total	С	Ν	0	S	0	1	4 0	
1	D	440	3445	2177	618	627	23	0	4	U	
1	C	C 440	Total	С	Ν	0	S	0	5	0	
1			3452	2181	621	627	23	0		0	
1	р	440	Total	С	Ν	0	S	0	5	0	
	440	3459	2185	624	627	23	0	5	U		

• Molecule 1 is a protein called ATP-dependent DNA helicase Q5.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	9	SER	-	expression tag	UNP O94762
А	10	MET	-	expression tag	UNP O94762
В	9	SER	-	expression tag	UNP O94762
В	10	MET	-	expression tag	UNP O94762
С	9	SER	-	expression tag	UNP O94762
С	10	MET	-	expression tag	UNP O94762
D	9	SER	-	expression tag	UNP O94762
D	10	MET	-	expression tag	UNP O94762

• Molecule 2 is a protein called Gluebody G5-006.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
0	V	194	Total	С	Ν	0	\mathbf{S}	0	1	0
	K	124	946	586	161	193	6	0	1	0
2	F	E 124	Total	С	Ν	0	S	0	1	0
			946	586	161	193	6	0		0
0	Б	F 124	Total	С	Ν	0	S	0	1	0
	2 F		946	586	161	193	6	0	1	0
0	С	194	Total	С	Ν	0	S	0	1	0
2 G	124	946	586	161	193	6	U		0	



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	187	Total O 187 187	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	186	Total O 186 186	0	0
5	С	193	Total O 193 193	0	0
5	D	186	Total O 186 186	0	0
5	K	78	Total O 78 78	0	0
5	Е	60	Total O 60 60	0	0
5	F	72	$\begin{array}{cc} \text{Total} & \text{O} \\ 72 & 72 \end{array}$	0	0
5	G	66	Total O 66 66	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 failed to run properly.

• Molecule 1: ATP-dependent DNA helicase Q5





C266 SER L275 SER L275 SER L275 SER F29 RE1 Y289 R2 Y289 R4 Y345 R51 T316 C51 G320 R65 Y344 T14 R329 T14 R3391 M143 R3391 M143 R3391 M144 R3391 M143 R3391 M143 R3391 M143 R440 S14 R440 S14 R440 S14 R43 S14

• Molecule 2: Gluebody G5-006

Chain K:	83%	14% •
SER MET ALA 41 41 41 7 7 7 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	F67 F87 V78 M82 M82 K86 K86 C35 C35 C35 C35 C35 C35 C35 C35 C35 C35	
• Molecule 2: Glueboo	dy G5-006	
Chain E:	83%	14% •
SER MET ALA 41 41 42 43 86 86 83 4 83 4 83 4 83 84 843	F67 T68 81 82 88 88 88 78 78 716 7116 7116 7125 7123 7123 7123	
• Molecule 2: Glueboo	dy G5-006	
Chain F:	82%	16% ·
SER MET ALA ALA ALA 41 43 43 66 711 712 713 73 86 73 86 73 86 73 86 73 86 73 86 73 87 74 74 74 74 74 74 74 74 74 74 74 74 74	K 43 F 67 F 67 F 67 F 67 F 68 M 82 C 96 C 96 C 96 C 116 C 116 C 116 C 116 C 123 C 124	
• Molecule 2: Glueboo	dy G5-006	
Chain G:	81%	17% •
SER MET ALA ALA V V V C L C L C L C C L C S 17 S 17 S 17 S 17 S 17 S S 17 S S 17 S S C S S R M MET MET MET MET MET MET A MET A MET A A A A A A A A A A A A A A A A A A A	M34 K43 A50 A50 A50 A50 M82 K86 M82 K86 K86 K86 C95 C95 C95 S116 S116 S112 S124	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	232.59Å 89.97Å 164.13Å	Depositor
a, b, c, α , β , γ	90.00° 110.06° 90.00°	Depositor
Resolution (Å)	77.69 - 2.00	Depositor
% Data completeness	97 6 (77 69-2 00)	Depositor
(in resolution range)	51.0 (11.05-2.00)	
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.45 (at 2.00 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.243 , 0.275	Depositor
Wilson B-factor $(Å^2)$	39.8	Xtriage
Anisotropy	0.067	Xtriage
L-test for twinning ²	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18647	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 61.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3908e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: ZN, SO4

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		Bo	nd lengths	Bo	ond angles
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.69	0/3531	0.79	1/4770~(0.0%)
1	В	0.71	1/3518~(0.0%)	0.80	0/4753
1	С	0.69	0/3535	0.80	0/4774
1	D	0.70	0/3535	0.79	0/4774
2	Ε	0.66	0/968	0.85	0/1314
2	F	0.69	0/968	0.86	0/1314
2	G	0.71	0/968	0.85	0/1314
2	K	0.70	0/968	0.87	0/1314
All	All	0.69	1/17991~(0.0%)	0.81	1/24327~(0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	158	GLU	CD-OE2	-5.01	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	180	ARG	CG-CD-NE	5.48	123.32	111.80

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.



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3455	0	3486	48	0
1	В	3445	0	3473	36	0
1	С	3452	0	3479	40	0
1	D	3459	0	3497	38	0
2	Е	946	0	887	9	0
2	F	946	0	887	12	0
2	G	946	0	887	14	0
2	Κ	946	0	887	13	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	А	5	0	0	0	0
4	В	5	0	0	0	0
4	С	5	0	0	0	0
4	D	5	0	0	0	0
5	А	187	0	0	8	0
5	В	186	0	0	6	0
5	С	193	0	0	9	0
5	D	186	0	0	6	0
5	Ε	60	0	0	1	0
5	F	72	0	0	2	0
5	G	66	0	0	2	0
5	K	78	0	0	5	0
All	All	18647	0	17483	209	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.

The worst 5 of 209 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:D:143:ASN:O	1:D:146:VAL:HG22	1.60	1.00
1:D:248:LYS:HG2	5:D:647:HOH:O	1.62	0.97
1:C:352:ARG:HD3	5:C:660:HOH:O	1.71	0.90
1:B:442:ARG:HG3	5:B:730:HOH:O	1.71	0.89
1:A:306:MET:HE1	1:A:323:VAL:HG21	1.62	0.82

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	Perce	ntiles
1	А	443/445~(100%)	432 (98%)	11 (2%)	0	100	100
1	В	442/445~(99%)	433~(98%)	9~(2%)	0	100	100
1	С	443/445~(100%)	430 (97%)	13 (3%)	0	100	100
1	D	443/445~(100%)	430~(97%)	13 (3%)	0	100	100
2	Е	123/127~(97%)	119 (97%)	4 (3%)	0	100	100
2	F	123/127~(97%)	120 (98%)	3~(2%)	0	100	100
2	G	123/127~(97%)	118 (96%)	5(4%)	0	100	100
2	K	123/127~(97%)	119 (97%)	4 (3%)	0	100	100
All	All	2263/2288~(99%)	2201 (97%)	62 (3%)	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	Perce	ntiles
1	А	369/373~(99%)	366~(99%)	3 (1%)	81	86
1	В	368/373~(99%)	364~(99%)	4 (1%)	73	78
1	С	370/373~(99%)	368 (100%)	2(0%)	88	92
1	D	370/373~(99%)	367~(99%)	3 (1%)	81	86
2	Ε	98/100~(98%)	95~(97%)	3~(3%)	40	40
2	F	98/100~(98%)	96~(98%)	2(2%)	55	58

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Mol	Chain	Analysed Rotameric Outliers		Percentiles		
2	G	98/100~(98%)	96~(98%)	2(2%)	55	58
2	Κ	98/100 (98%)	97~(99%)	1 (1%)	76	81
All	All	1869/1892~(99%)	1849 (99%)	20 (1%)	73	78

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5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
2	Ε	68	THR
2	F	95	CYS
2	G	95	CYS
2	G	68	THR
1	В	409	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such side chains are listed below:

Mol	Chain	Res	Type
1	D	302	GLN
2	Κ	120	GLN
2	G	120	GLN
2	Κ	81	GLN
2	Е	3	GLN

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)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.



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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	SO4	С	502	-	4,4,4	0.30	0	6,6,6	0.22	0
4	SO4	D	502	-	4,4,4	0.12	0	6,6,6	0.27	0
4	SO4	А	502	-	4,4,4	0.29	0	6,6,6	0.12	0
4	SO4	В	502	-	4,4,4	0.31	0	6,6,6	0.23	0

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 (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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

