

Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 03:39 PM EDT

PDB ID	:	7UWI
Title	:	Structure of beta-catenin in complex with FP01567, a Helicon Polypeptide
Authors	:	Brennan, M.; Agarwal, S.; Thomson, T.; Wahl, S.; Ramirez, J.; Verdine, G.;
		McGee, J.
Deposited on	:	2022-05-03
Resolution	:	2.32 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:

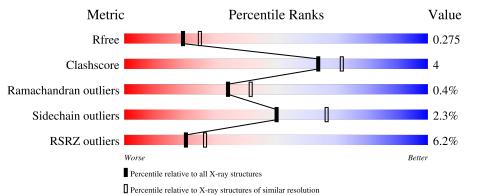
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	:::::::::::::::::::::::::::::::::::::::	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 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 2.32 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5974(2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	$5855\ (2.34-2.30)$

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 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	А	521	6% 85%		11% •
2	F	16	19%	12%	12%

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 criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	А	701	-	-	-	Х
4	GOL	А	702	-	-	-	Х
4	GOL	А	703	-	-	-	Х
4	GOL	А	706	-	-	-	Х
4	GOL	А	707	-	-	-	Х



7UWI

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4073 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.

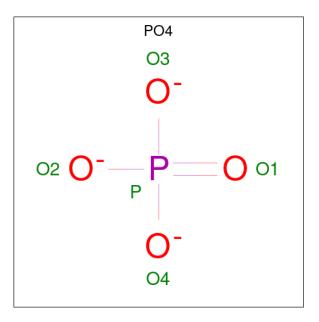
• Molecule 1 is a protein called Catenin beta-1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	505	Total	C 2410	N 609	O 706	S 26	0	1	0
			3849	2419	698	700	20			

• Molecule 2 is a protein called Helicon Polypeptide FP01567.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	F	14	Total 109	C 68	N 22	0 17	${ m S} { m 2}$	0	0	1

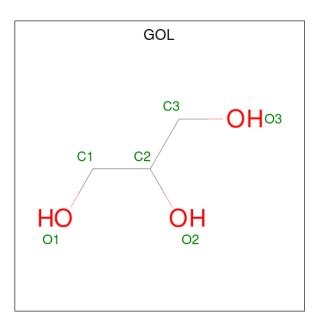
• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 5	0 4	Р 1	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

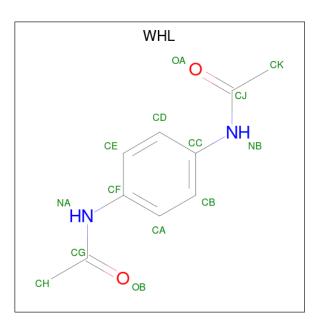




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	А	1	TotalCO633	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 5 is N,N'-(1,4-phenylene)diacetamide (three-letter code: WHL) (formula: $C_{10}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).





M	ol	Chain	Residues	Atoms				ZeroOcc	AltConf
5		\mathbf{F}	1	Total 14	C 10	N 2	O 2	0	0

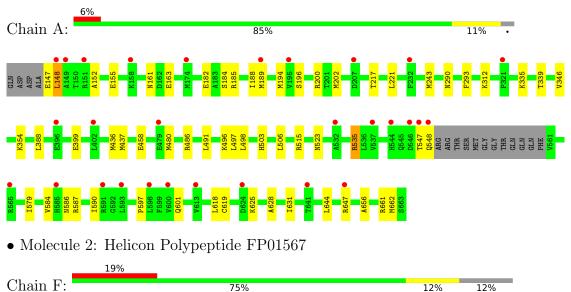
• Molecule 6 is water.

M	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
6		А	59	Total O 59 59	0	0
6	1	F	1	Total O 1 1	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: Catenin beta-1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	49.68Å 91.81Å 113.35Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.34 - 2.32	Depositor
Resolution (A)	71.34 - 2.32	EDS
% Data completeness	99.7 (71.34-2.32)	Depositor
(in resolution range)	99.7(71.34-2.32)	EDS
R _{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.72 (at 2.32 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20_4444	Depositor
D D.	0.236 , 0.278	Depositor
R, R_{free}	0.234 , 0.275	DCC
R_{free} test set	1126 reflections (4.88%)	wwPDB-VP
Wilson B-factor $(Å^2)$	51.8	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 40.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4073	wwPDB-VP
Average B, all atoms $(Å^2)$	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.65% of the height of the origin peak. No significant pseudotranslation is detected.

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: GOL, WHL, NH2, PO4 $\,$

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		lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.24	0/3905	0.45	0/5300	
2	F	0.26	0/111	0.41	0/150	
All	All	0.24	0/4016	0.45	0/5450	

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	3849	0	4001	34	0
2	F	109	0	97	1	0
3	А	5	0	0	0	0
4	А	36	0	48	2	0
5	F	14	0	0	0	0
6	А	59	0	0	2	0
6	F	1	0	0	0	0
All	All	4073	0	4146	34	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 4.



Atom-1	Atom-2	Interatomic	Clash
	1100111 2	distance (Å)	overlap (Å)
1:A:498:LEU:HB3	1:A:535:ARG:HG2	1.81	0.62
1:A:312:LYS:HD3	1:A:346:VAL:HG12	1.83	0.61
1:A:335:LYS:HD2	2:F:10:LEU:HD12	1.85	0.59
1:A:188:ILE:HG23	1:A:194:MET:HG2	1.86	0.58
1:A:436:MET:HE1	6:A:805:HOH:O	2.05	0.57
1:A:628:ALA:HB1	1:A:662:MET:HA	1.91	0.53
1:A:217:THR:O	1:A:221:LEU:HD12	2.09	0.52
1:A:497:LEU:HD22	1:A:506:LEU:HD21	1.91	0.52
1:A:196:SER:O	1:A:200:ARG:HG3	2.10	0.52
1:A:148:LEU:HA	1:A:152:ALA:HB3	1.91	0.52
1:A:354:LYS:HG2	1:A:388:LEU:HD23	1.92	0.52
1:A:586:ASN:O	1:A:590:ILE:HG13	2.10	0.51
1:A:161:ASN:HB3	1:A:200:ARG:NH2	2.26	0.50
1:A:486:ARG:O	4:A:702:GOL:O1	2.28	0.49
1:A:491:LEU:HB2	4:A:702:GOL:H11	1.94	0.48
1:A:182:GLU:OE1	1:A:185:ARG:NH1	2.47	0.48
1:A:486:ARG:HB2	1:A:523:ASN:HD21	1.79	0.47
1:A:619:CYS:O	1:A:661:ARG:NH1	2.47	0.47
1:A:515:ARG:HG3	1:A:579:ILE:HD12	1.97	0.47
1:A:161:ASN:HB3	1:A:200:ARG:HH22	1.81	0.46
1:A:597:PRO:O	1:A:601:GLN:HG2	2.16	0.45
1:A:644:LEU:HD21	1:A:656:ALA:HB2	1.99	0.45
1:A:458:GLU:OE2	1:A:503:HIS:ND1	2.51	0.43
1:A:335:LYS:HE3	1:A:335:LYS:HB2	1.70	0.43
1:A:618:LEU:HD22	1:A:631:ILE:HG12	2.02	0.42
1:A:584:VAL:HG22	1:A:587:ARG:NH2	2.34	0.42
1:A:399:GLU:HG3	1:A:437:MET:HE3	2.02	0.42
1:A:202:MET:HG2	1:A:243:MET:SD	2.59	0.41
1:A:625:LYS:HE3	1:A:625:LYS:HB2	1.78	0.41
1:A:184:SER:O	1:A:188:ILE:HG13	2.20	0.41
1:A:148:LEU:HD23	1:A:152:ALA:HB3	2.02	0.41
1:A:339:THR:HG23	6:A:813:HOH:O	2.20	0.41
1:A:644:LEU:HA	1:A:644:LEU:HD23	1.78	0.41
1:A:290:ASN:HB3	1:A:293:PHE:HB3	2.03	0.40

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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 Po		Perce	Percentiles		
1	А	502/521~(96%)	493 (98%)	7 (1%)	2~(0%)	34	41
2	F	12/16~(75%)	11 (92%)	1 (8%)	0	100	100
All	All	514/537~(96%)	504 (98%)	8 (2%)	2 (0%)	34	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	148	LEU
1	А	547	THR

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	alysed Rotameric Outliers		Percentiles		
1	А	419/431~(97%)	410 (98%)	9~(2%)	53 70		
2	F	11/12~(92%)	10 (91%)	1 (9%)	9 11		
All	All	430/443~(97%)	420 (98%)	10 (2%)	50 66		

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	147	GLU
1	А	155	GLU
1	А	163	GLU
1	А	189	MET

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Mol	Chain	Res	Type
1			÷ =
1	A	480	MET
1	А	496	LYS
1	А	535	ARG
1	А	548	GLN
1	А	647	ARG
2	F	4	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	А	353	ASN
1	А	523	ASN
1	А	601	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)

8 ligands 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	ol Type Chain Res Li		Link	Bo	ond leng	\mathbf{ths}	Bond angles			
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	GOL	А	702	-	$5,\!5,\!5$	0.91	0	$5,\!5,\!5$	1.00	0
4	GOL	А	705	-	$5,\!5,\!5$	0.92	0	$5,\!5,\!5$	1.00	0
4	GOL	А	703	-	$5,\!5,\!5$	0.91	0	$5,\!5,\!5$	1.00	0
4	GOL	А	706	-	$5,\!5,\!5$	0.92	0	$5,\!5,\!5$	0.99	0
4	GOL	А	707	-	$5,\!5,\!5$	0.92	0	$5,\!5,\!5$	0.99	0
3	PO4	А	701	-	4,4,4	0.92	0	$6,\!6,\!6$	0.43	0
5	WHL	F	101	2	$14,\!14,\!14$	0.59	0	18,18,18	1.37	2 (11%)
4	GOL	А	704	-	$5,\!5,\!5$	0.90	0	$5,\!5,\!5$	0.98	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
4	GOL	А	702	-	-	0/4/4/4	-
4	GOL	А	705	-	-	0/4/4/4	-
4	GOL	А	703	-	-	0/4/4/4	-
4	GOL	А	706	-	-	3/4/4/4	-
4	GOL	А	707	-	-	0/4/4/4	-
5	WHL	F	101	2	-	0/8/8/8	0/1/1/1
4	GOL	А	704	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	F	101	WHL	CK-CJ-NB	3.34	119.88	114.98
5	F	101	WHL	OA-CJ-CK	-2.82	116.83	122.06

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	704	GOL	C1-C2-C3-O3
4	А	706	GOL	O1-C1-C2-C3
4	А	704	GOL	O2-C2-C3-O3
4	А	706	GOL	O2-C2-C3-O3
4	А	706	GOL	O1-C1-C2-O2

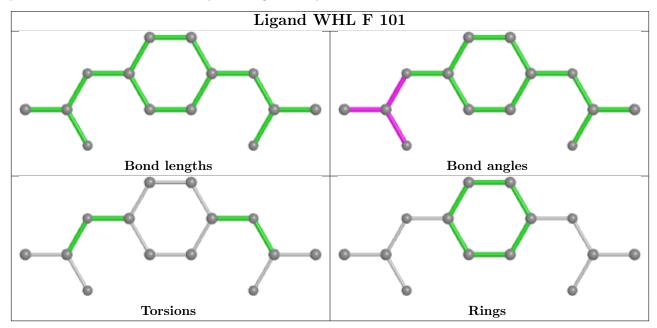


There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	702	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	505/521~(96%)	0.65	29 (5%) 23 30	33, 61, 83, 100	0
2	F	13/16~(81%)	1.10	3(23%) 0 1	57, 74, 99, 100	0
All	All	518/537~(96%)	0.66	32 (6%) 20 26	33, 61, 84, 100	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	149	ALA	5.9
1	А	547	THR	5.5
1	А	148	LEU	5.0
1	А	565	ARG	4.5
1	А	151	ARG	4.2
1	А	548	GLN	3.8
1	А	598	LEU	3.6
1	А	174	MET	3.5
1	А	585	HIS	3.4
2	F	4	ARG	3.3
1	А	600	VAL	3.1
1	А	647	ARG	2.9
1	А	396	GLU	2.9
1	А	613	VAL	2.8
1	А	532	ALA	2.8
1	А	544	HIS	2.8
2	F	3	HIS	2.7
1	А	546	ASP	2.6
1	А	195	VAL	2.5
1	А	537	VAL	2.5
1	А	402	LEU	2.4
1	А	207	ASP	2.3
1	А	593	LEU	2.3
1	А	189	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	А	624	ASP	2.2
1	А	591	ARG	2.2
2	F	15	VAL	2.2
1	А	641	THR	2.1
1	А	479	GLU	2.1
1	А	321	PRO	2.1
1	А	158	LYS	2.1
1	А	232	PHE	2.0

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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.

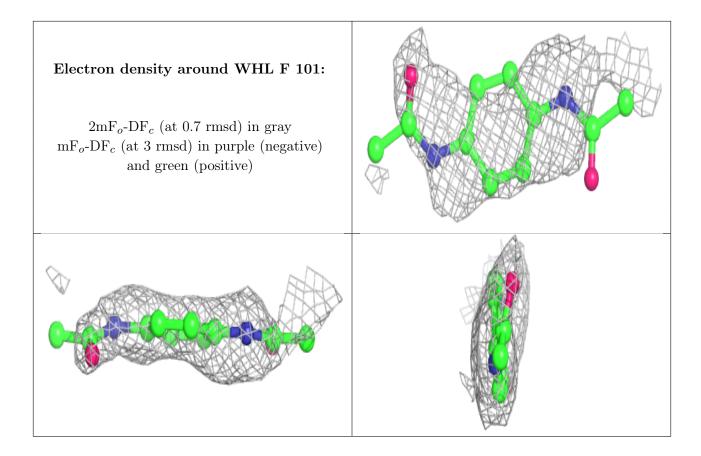
6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
4	GOL	А	702	6/6	0.37	0.91	59,79,84,88	0
4	GOL	А	703	6/6	0.47	0.47	74,93,96,108	0
4	GOL	А	704	6/6	0.55	0.40	77,85,91,91	0
4	GOL	А	706	6/6	0.55	0.71	66,75,89,106	0
4	GOL	А	705	6/6	0.62	0.29	72,76,85,104	0
4	GOL	А	707	6/6	0.65	0.78	79,80,89,101	0
5	WHL	F	101	14/14	0.69	0.33	91,99,106,107	0
3	PO4	А	701	5/5	0.79	0.85	69,94,113,118	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

