

Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 11:36 am BST

PDB ID 5LWF

> Title Structure of a single domain camelid antibody fragment cAb-G10S in complex

> > with the BlaP beta-lactamase from Bacillus licheniformis

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Resolution 2.56 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

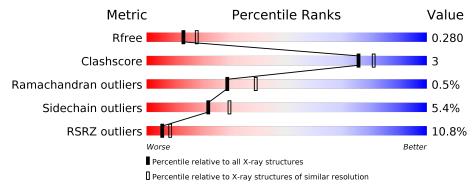
Validation Pipeline (wwPDB-VP) 2.11

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 2.56 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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 on 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	273	85%		9%	• 5%
1	В	273	16%		7%	• 5%
2	С	131	75%	17%		• 7%
2	D	131	18%	12%	•	10%

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	С	202	-	_	_	X



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5927 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 Beta-lactamase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	259	Total 2019	C 1266	N 349	O 401	S 3	0	0	0
1	В	258	Total 2014	C 1263	N 348	O 400	S 3	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197A	PRO	-	insertion	UNP P00808
A	197B	GLY	-	insertion	UNP P00808
A	296	GLY	-	expression tag	UNP P00808
A	297	PRO	_	expression tag	UNP P00808
A	298	HIS	_	expression tag	UNP P00808
A	299	HIS	_	expression tag	UNP P00808
A	300	HIS	-	expression tag	UNP P00808
A	301	HIS	-	expression tag	UNP P00808
A	302	HIS	-	expression tag	UNP P00808
В	197A	PRO	-	insertion	UNP P00808
В	197B	GLY	_	insertion	UNP P00808
В	296	GLY	-	expression tag	UNP P00808
В	297	PRO	_	expression tag	UNP P00808
В	298	HIS	-	expression tag	UNP P00808
В	299	HIS	-	expression tag	UNP P00808
В	300	HIS	=	expression tag	UNP P00808
В	301	HIS	-	expression tag	UNP P00808
В	302	HIS	-	expression tag	UNP P00808

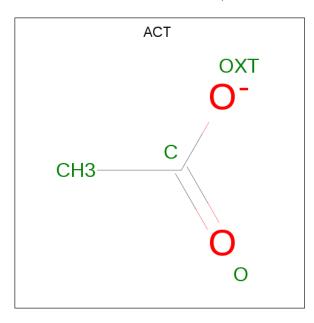
• Molecule 2 is a protein called Camelid heavy-chain antibody variable fragment cAb-G10S.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	С	122	Total 948	C 599	N 163	O 182	S 4	0	0	0



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	D	110	Total	С	N	О	S	0	0	0
	ש	110	925	584	159	178	4	0		0

 \bullet Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $\mathrm{C_2H_3O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	С	1	Total C O 4 2 2	0	0
3	С	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	Total O 1 1	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Beta-lactamase Chain A: 85% • 5% • Molecule 1: Beta-lactamase Chain B: 86% • Molecule 2: Camelid heavy-chain antibody variable fragment cAb-G10S Chain C: • Molecule 2: Camelid heavy-chain antibody variable fragment cAb-G10S Chain D: 10%







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	47.28Å 121.69Å 137.03Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.50 - 2.56	Depositor
resolution (11)	45.50 - 2.56	EDS
% Data completeness	93.9 (40.50-2.56)	Depositor
(in resolution range)	$94.4 \ (45.50 - 2.56)$	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.34 \; (at \; 2.58 \text{Å})$	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.215 , 0.242	Depositor
it, it free	0.246 , 0.280	DCC
R_{free} test set	1231 reflections (4.98%)	wwPDB-VP
Wilson B-factor (\mathring{A}^2)	34.2	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 41.2	EDS
L-test for twinning ²	$ < L > = 0.45, < L^2> = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5927	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: ACT

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).

Mal	Chain	Bond	lengths	Bond angles		
Mol		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.36	0/2050	0.64	1/2777 (0.0%)	
1	В	0.36	0/2045	0.64	0/2770	
2	С	0.35	0/972	0.61	0/1317	
2	D	0.37	0/948	0.60	0/1283	
All	All	0.36	0/6015	0.63	1/8147 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	A	197	ASP	CA-CB-CG	-5.38	101.56	113.40

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	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	A	2019	0	2028	12	0
1	В	2014	0	2026	8	0
2	С	948	0	900	9	0
2	D	925	0	873	7	0
3	A	8	0	6	0	0
3	С	8	0	6	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4	0	3	0	0
4	С	1	0	0	0	0
All	All	5927	0	5842	36	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 3.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1Atom-21:A:109:THR:HG211:A:133:ALA:HB31:A:44:LEU:HD211:A:278:LEU:HD111:B:109:THR:HG211:B:133:ALA:HB32:D:71:PHE:HD12:D:72:ALA:H1:A:106:ASN:HB31:A:109:THR:CG21:A:183:ALA:O1:A:187:VAL:HG132:D:63:TYR:CE12:D:71:PHE:HB2	1.50 1.58 1.70 1.38	0.94 0.83 0.73
1:A:44:LEU:HD21 1:A:278:LEU:HD11 1:B:109:THR:HG21 1:B:133:ALA:HB3 2:D:71:PHE:HD1 2:D:72:ALA:H 1:A:106:ASN:HB3 1:A:109:THR:CG2 1:A:183:ALA:O 1:A:187:VAL:HG13	1.58 1.70 1.38	0.83
1:B:109:THR:HG21 1:B:133:ALA:HB3 2:D:71:PHE:HD1 2:D:72:ALA:H 1:A:106:ASN:HB3 1:A:109:THR:CG2 1:A:183:ALA:O 1:A:187:VAL:HG13	1.70 1.38	
2:D:71:PHE:HD1 2:D:72:ALA:H 1:A:106:ASN:HB3 1:A:109:THR:CG2 1:A:183:ALA:O 1:A:187:VAL:HG13	1.38	0.73
1:A:106:ASN:HB3 1:A:109:THR:CG2 1:A:183:ALA:O 1:A:187:VAL:HG13		
1:A:183:ALA:O 1:A:187:VAL:HG13	0.07	0.69
	2.27	0.63
9.D.69.TVD.CE1 9.D.71.DHE.HD9	2.02	0.60
	2.36	0.59
2:C:23:LEU:HD12 2:C:84:LEU:HD23	1.85	0.57
2:D:69:GLY:H 2:D:71:PHE:HD2	1.53	0.56
1:B:183:ALA:O 1:B:187:VAL:HG13	2.05	0.56
2:C:37:MET:HG3 2:C:82:VAL:HG11	1.88	0.55
1:A:106:ASN:HB3 1:A:109:THR:HG23	1.89	0.53
1:B:40:PHE:HB2 1:B:278:LEU:HD13	1.91	0.52
2:C:26:ALA:HA 2:C:81:THR:HG22	1.91	0.51
1:A:33:PHE:CE1 1:A:46:ILE:HD13	2.48	0.48
2:D:23:LEU:HD12 2:D:84:LEU:HD23	1.96	0.47
2:D:26:ALA:HA 2:D:81:THR:HG22	1.97	0.47
1:B:45:GLY:HA3 1:B:66:PHE:HE2	1.80	0.47
1:A:231:VAL:HG22 1:A:250:ILE:HG23	1.97	0.46
2:D:94:THR:HG23 2:D:125:THR:HA	1.99	0.45
1:A:119:LEU:HD21 1:A:141:GLN:HG3	1.98	0.45
2:D:75:ARG:HB3 2:D:82:VAL:HG13	2.00	0.44
2:C:54:ILE:HD13 2:C:75:ARG:HG3	1.99	0.44
1:B:187:VAL:HB 1:B:260:VAL:HG22	2.00	0.44
2:C:94:THR:HG23 2:C:125:THR:HA	1.99	0.44
1:B:45:GLY:HA3 1:B:66:PHE:CE2	2.54	0.43
1:A:261:LEU:HD11 1:A:263:VAL:CG2	2.47	0.43
1:B:119:LEU:HD21 1:B:141:GLN:HG3	2.00	0.43
1:B:255:LYS:HD3 1:B:255:LYS:H	1.85	0.42
2:C:106:ARG:HD3 2:C:114:THR:O	2.19	0.42
2:C:90:LYS:HG2 2:C:91:PRO:HD2	2.02	0.42



Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
1:A:197(A):PRO:CG	1:A:197(A):PRO:O	2.67	0.42
2:C:63:TYR:HB2	2:C:68:LYS:HG2	2.01	0.42
1:A:225:VAL:CG1	1:A:229:TRP:HB2	2.50	0.41
1:A:197(A):PRO:HG2	1:A:197(A):PRO:O	2.20	0.41
2:C:101:ALA:HB3	2:C:117:TYR:HB2	2.02	0.41

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	entiles
1	A	$257/273 \ (94\%)$	250 (97%)	5 (2%)	2 (1%)	19	27
1	В	256/273~(94%)	251 (98%)	4 (2%)	1 (0%)	34	45
2	C	$120/131 \; (92\%)$	115 (96%)	5 (4%)	0	100	100
2	D	114/131 (87%)	106 (93%)	7 (6%)	1 (1%)	17	24
All	All	747/808 (92%)	722 (97%)	21 (3%)	4 (0%)	29	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	72	ALA
1	A	197(B)	GLY
1	В	103	VAL
1	A	103	VAL

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	Chain Analysed Rotameric Outliers		Percentiles		
1	A	$217/230 \ (94\%)$	210 (97%)	7 (3%)	39	51
1	В	$217/230 \ (94\%)$	205 (94%)	12 (6%)	21	29
2	С	96/105~(91%)	88 (92%)	8 (8%)	11	14
2	D	94/105~(90%)	87 (93%)	7 (7%)	13	18
All	All	624/670 (93%)	590 (95%)	34 (5%)	22	29

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	56	THR
1	A	163	GLU
1	A A	178	GLN VAL
1	A	187	VAL
1	A	233	ASP
1	A	261	LEU
1	В	35	LYS
1	В	56	THR
1	В	68	PHE
1	В	109	THR
1	В	159	VAL
1	В	163	GLU
1	В	178	GLN
1	В	187	VAL
1	В	233	ASP
1	В	255	LYS
1	В	268	ASP
1	B C	273	LYS LEU
2	С	14	LEU
2	С	15	VAL
2	C	30	ARG
2	C C C C C D	31	THR
2	С	67	VAL
2	С	68	LYS
2	С	73	PHE
2	С	106	ARG
2	D	15	VAL
2	D	46	LYS
2	D	70	ARG



Mol	Chain	Res	Type
2	D	73	PHE
2	D	75	ARG
2	D	92	GLU
2	D	106	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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).

Mal	Mol Type Chain I		Res Link		Chain Bond lengths		${f gths}$	Bond angles		
MIOI	Type	Chain	1162	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	ACT	A	402	-	1,3,3	4.90	1 (100%)	0,3,3	0.00	-
3	ACT	С	201	-	1,3,3	4.98	1 (100%)	0,3,3	0.00	-
3	ACT	С	202	-	1,3,3	4.89	1 (100%)	0,3,3	0.00	-



Mol	Т	Chain	Res	Link	В	ond len	$_{ m gths}$	В	ond ang	gles
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	ACT	A	401	-	1,3,3	4.83	1 (100%)	0,3,3	0.00	-
3	ACT	D	201	_	1,3,3	4.86	1 (100%)	0,3,3	0.00	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
3	С	201	ACT	СН3-С	4.98	1.55	1.48
3	A	402	ACT	СН3-С	4.90	1.55	1.48
3	С	202	ACT	СН3-С	4.89	1.55	1.48
3	D	201	ACT	СН3-С	4.86	1.54	1.48
3	A	401	ACT	СН3-С	4.83	1.54	1.48

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)

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	<RSRZ $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	$259/273 \ (94\%)$	0.36	8 (3%) 49 58	21, 44, 78, 106	0
1	В	258/273 (94%)	0.91	44 (17%) 1 1	19, 61, 124, 152	0
2	С	122/131 (93%)	0.31	6 (4%) 29 37	16, 44, 70, 81	0
2	D	118/131 (90%)	1.26	24 (20%) 1 1	22, 72, 106, 116	0
All	All	757/808 (93%)	0.68	82 (10%) 5 8	16, 50, 106, 152	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	256	GLY	11.2
2	D	78	ALA	7.6
1	В	291	ASN	6.1
1	В	229	TRP	5.9
2	D	79	LYS	5.8
1	В	288	LYS	5.6
1	В	284	LYS	5.4
1	В	290	LEU	5.1
1	В	277	LYS	5.1
1	В	287	MET	4.8
2	D	120	GLN	4.7
2	С	120	GLN	4.6
1	В	208	ILE	4.4
1	В	40	PHE	4.4
1	В	252	PRO	4.1
1	В	32	ASP	4.1
2	D	77	ASN	4.0
2	D	8	GLN	4.0
2	D	15	VAL	4.0
2	D	16	GLN	3.9
1	В	255	LYS	3.9



Continued from previous page...

Mol 1	Chain	${ m Res}$	Type	RZRZ
1 1				RSRZ
	В	289	ALA	3.9
2	D	81	THR	3.8
2	С	44	PRO	3.8
2	D	89	LEU	3.8
	В	251	TRP	3.8
1	В	31	ASP	3.7
1	В	254	PRO	3.5
1	В	225	VAL	3.5
2	D	6	GLN	3.5
1	В	250	ILE	3.5
1	Α	255	LYS	3.4
1	В	280	ALA	3.4
2	С	92	GLU	3.4
1	Α	254	PRO	3.3
2	D	11	GLY	3.3
1	В	35	LYS	3.2
2	D	44	PRO	3.0
1	В	226	PRO	3.0
1	В	227	ASP	3.0
1	В	259	VAL	3.0
2	D	26	ALA	2.9
2	С	14	LEU	2.9
1	В	278	LEU	2.8
2	D	122	THR	2.8
1	A	51	THR	2.8
1	В	230	GLU	2.8
1	В	53	THR	2.8
1	A	271	ASP	2.7
1	В	285	VAL	2.7
1	В	196	GLU	2.7
1	В	34	ALA	2.6
2	D	98	TYR	2.6
2	D	22	ARG	2.6
1	В	224	GLY	2.6
2	D	23	LEU	2.6
1	В	39	GLN	2.6
1	A	114	ASP	2.6
1	В	260	VAL	2.5
2	С	89	LEU	2.5
1	В	42	ALA	2.5
1	В	55	ARG	2.4
2	D	126	VAL	2.4



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Mol	Chain	Res	Type	RSRZ
1	A	31	ASP	2.3
1	A	227	ASP	2.3
2	D	45	GLY	2.3
2	D	25	CYS	2.3
1	В	201	SER	2.3
2	D	24	SER	2.3
1	В	44	LEU	2.3
1	В	257	ASP	2.2
1	В	195	LEU	2.2
2	D	80	ASN	2.2
1	В	38	GLU	2.2
1	В	268	ASP	2.2
2	D	124	VAL	2.2
1	В	206	LEU	2.2
1	A	228	GLY	2.1
1	В	223	ALA	2.1
1	В	212	LYS	2.1
2	С	68	LYS	2.1
2	D	56	PRO	2.0

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 carbohydrates 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	${f Res}$	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	ACT	С	202	4/4	0.69	0.41	49,50,50,52	0
3	ACT	A	401	4/4	0.89	0.24	55,56,56,56	0
3	ACT	С	201	4/4	0.92	0.24	33,34,35,35	0
3	ACT	A	402	4/4	0.94	0.15	33,33,34,34	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q<0.9
3	ACT	D	201	4/4	0.97	0.16	40,40,40,41	0

6.5 Other polymers (i)

There are no such residues in this entry.

