



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:55 pm GMT

PDB ID : 5OE7  
Title : Structure of OTULIN bound to the Met1-linked diubiquitin activity probe  
Authors : Elliott, P.R.; Komander, D.  
Deposited on : 2017-07-07  
Resolution : 2.95 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtrriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

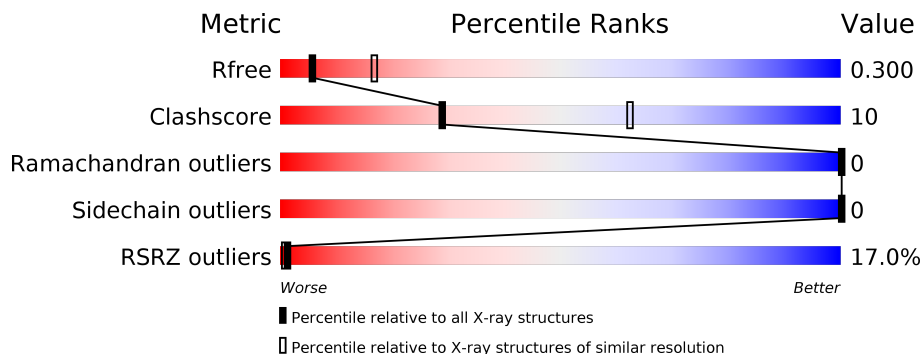
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	111664	2641 (3.00-2.92)
Clashscore	122126	2988 (3.00-2.92)
Ramachandran outliers	120053	2892 (3.00-2.92)
Sidechain outliers	120020	2895 (3.00-2.92)
RSRZ outliers	108989	2527 (3.00-2.92)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	
2	B	146	

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
2	DHA	B	76	-	X	-	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3077 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 Ubiquitin thioesterase otulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2019	1294	334	378	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	-	expression tag	UNP Q96BN8
A	79	PRO	-	expression tag	UNP Q96BN8

- Molecule 2 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1058	668	176	212	2	0	0	0

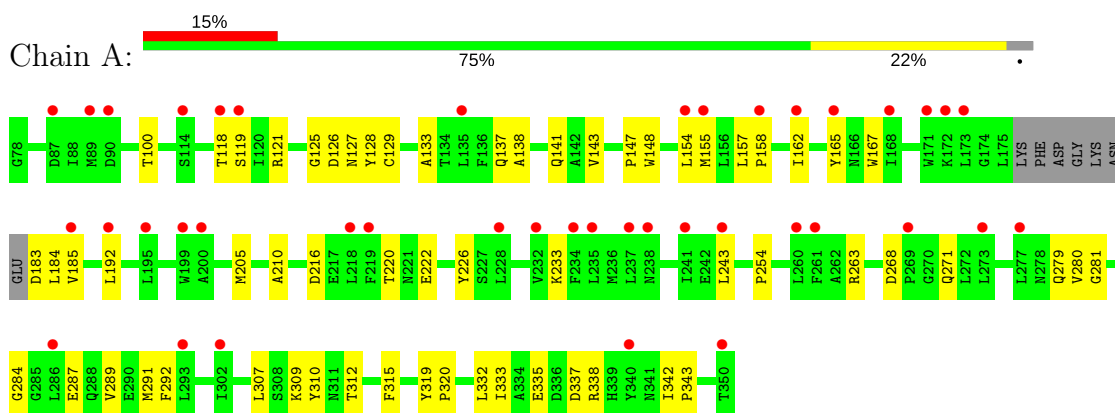
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	DHA	GLY	conflict	UNP P0CG48

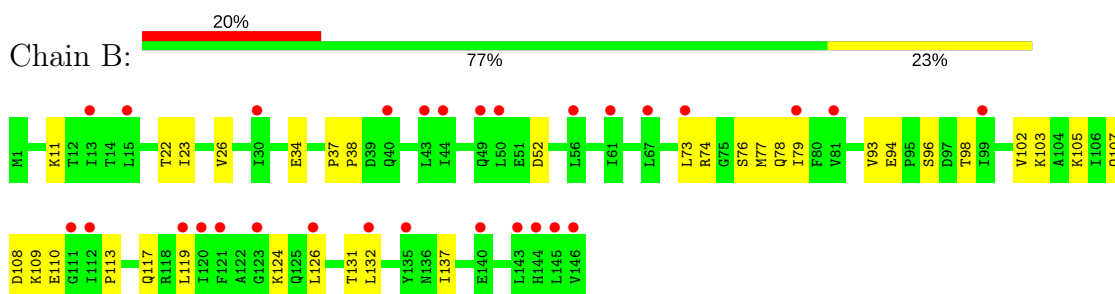
### 3 Residue-property plots

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: Ubiquitin thioesterase otulin



#### • Molecule 2: Polyubiquitin-C



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.14Å 101.14Å 277.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.43 – 2.95 54.43 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.43-2.95) 100.0 (54.43-2.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.96Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.223 , 0.309 0.231 , 0.300	Depositor DCC
$R_{free}$ test set	619 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.8	Xtrriage
Anisotropy	0.573	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 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: DHA

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	1.00	0/2067	1.03	0/2831
2	B	0.96	0/1065	1.08	0/1455
All	All	0.99	0/3132	1.05	0/4286

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	A	2019	0	1859	41	0
2	B	1058	0	1001	26	0
All	All	3077	0	2860	62	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 10.

All (62) 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)
2:B:74:ARG:NH2	2:B:94:GLU:OE2	2.04	0.90
2:B:77:MET:HG2	2:B:93:VAL:CG2	2.14	0.78
1:A:154:LEU:HG	1:A:192:LEU:HD21	1.65	0.76
1:A:162:ILE:HD13	1:A:185:VAL:HG22	1.68	0.75
1:A:333:ILE:HD11	1:A:343:PRO:HB3	1.70	0.72
1:A:158:PRO:O	1:A:162:ILE:HD12	1.91	0.70
2:B:94:GLU:HG2	2:B:96:SER:OG	1.93	0.69
2:B:77:MET:HG2	2:B:93:VAL:HG22	1.76	0.67
2:B:98:THR:HG22	2:B:131:THR:HG22	1.75	0.67
1:A:133:ALA:HB1	1:A:332:LEU:HD22	1.78	0.64
2:B:105:LYS:O	2:B:108:ASP:N	2.32	0.63
1:A:127:ASN:HA	2:B:76:DHA:O	1.99	0.63
1:A:205:MET:CE	1:A:210:ALA:HB1	2.29	0.62
2:B:11:LYS:NZ	2:B:34:GLU:OE1	2.24	0.62
1:A:205:MET:HE1	1:A:210:ALA:HB1	1.84	0.60
1:A:126:ASP:O	1:A:127:ASN:HB2	2.02	0.60
1:A:233:LYS:CE	1:A:280:VAL:HB	2.32	0.59
1:A:233:LYS:HE2	1:A:280:VAL:HB	1.84	0.58
1:A:263:ARG:NH1	1:A:287:GLU:OE1	2.37	0.58
2:B:77:MET:HG2	2:B:93:VAL:HG23	1.85	0.57
1:A:222:GLU:O	1:A:226:TYR:HD1	1.86	0.57
1:A:333:ILE:HD11	1:A:343:PRO:CB	2.34	0.57
1:A:310:TYR:HA	1:A:315:PHE:CD1	2.40	0.56
1:A:157:LEU:C	1:A:157:LEU:HD23	2.25	0.56
2:B:132:LEU:HD22	2:B:137:ILE:HG21	1.88	0.56
1:A:183:ASP:CG	1:A:184:LEU:N	2.59	0.55
2:B:23:ILE:HB	2:B:52:ASP:HA	1.89	0.54
1:A:289:VAL:O	1:A:292:PHE:HB2	2.08	0.54
2:B:94:GLU:HG3	2:B:96:SER:H	1.73	0.53
1:A:216:ASP:O	1:A:220:THR:HG23	2.09	0.52
1:A:307:LEU:HD12	1:A:335:GLU:HG2	1.91	0.52
1:A:155:MET:O	1:A:158:PRO:HD2	2.08	0.52
1:A:128:TYR:CZ	1:A:281:GLY:HA3	2.45	0.51
1:A:128:TYR:O	1:A:129:CYS:C	2.50	0.50
2:B:109:LYS:O	2:B:110:GLU:HG2	2.12	0.50
1:A:165:TYR:HB3	1:A:167:TRP:CE2	2.46	0.49
2:B:94:GLU:CG	2:B:96:SER:OG	2.58	0.49
1:A:280:VAL:HA	1:A:284:GLY:O	2.12	0.49
1:A:125:GLY:HA3	2:B:78:GLN:HB2	1.96	0.48
2:B:102:VAL:O	2:B:103:LYS:C	2.51	0.48
2:B:107:GLN:NE2	2:B:113:PRO:HA	2.28	0.48
1:A:141:GLN:O	1:A:143:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:O	1:A:271:GLN:N	2.49	0.46
1:A:338:ARG:HD3	2:B:93:VAL:HA	1.98	0.45
1:A:205:MET:CE	1:A:210:ALA:CB	2.94	0.45
1:A:121:ARG:HB2	1:A:342:ILE:HB	1.98	0.45
2:B:103:LYS:HA	2:B:117:GLN:OE1	2.17	0.45
2:B:37:PRO:HA	2:B:38:PRO:HD3	1.83	0.45
2:B:22:THR:O	2:B:26:VAL:HG23	2.17	0.44
1:A:100:THR:HG21	2:B:108:ASP:OD1	2.18	0.43
1:A:137:GLN:O	1:A:138:ALA:C	2.55	0.43
1:A:309:LYS:O	1:A:312:THR:OG1	2.25	0.42
2:B:79:ILE:HD11	2:B:93:VAL:HG11	2.00	0.42
1:A:147:PRO:O	1:A:148:TRP:C	2.55	0.42
1:A:118:THR:HG23	1:A:119:SER:OG	2.20	0.42
1:A:319:TYR:HA	1:A:320:PRO:HA	1.95	0.41
1:A:243:LEU:HD22	1:A:254:PRO:HD2	2.02	0.41
1:A:291:MET:O	1:A:292:PHE:C	2.59	0.41
2:B:124:LYS:O	2:B:126:LEU:CD2	2.69	0.41
1:A:337:ASP:HB2	2:B:73:LEU:HD21	2.02	0.40
2:B:119:LEU:O	2:B:126:LEU:HG	2.22	0.40
1:A:279:GLN:N	1:A:279:GLN:OE1	2.54	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	262/273 (96%)	247 (94%)	15 (6%)	0	100	100
2	B	143/146 (98%)	133 (93%)	10 (7%)	0	100	100
All	All	405/419 (97%)	380 (94%)	25 (6%)	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	200/242 (83%)	200 (100%)	0	100	100
2	B	108/132 (82%)	108 (100%)	0	100	100
All	All	308/374 (82%)	308 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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](#)

1 non-standard protein/DNA/RNA residue is 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DHA	B	76	1,2	4,4,5	2.93	3 (75%)	2,4,6	4.35	2 (100%)

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
2	DHA	B	76	1,2	-	0/0/2/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	76	DHA	C-CA	2.55	1.49	1.45
2	B	76	DHA	CB-CA	3.34	1.51	1.34
2	B	76	DHA	CA-N	3.59	1.44	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	DHA	O-C-CA	-4.39	117.34	125.47
2	B	76	DHA	CB-CA-N	-4.32	115.19	125.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	76	DHA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	266/273 (97%)	1.00	41 (15%) <b>2</b>   <b>1</b>	24, 45, 66, 85	0
2	B	145/146 (99%)	0.89	29 (20%) <b>1</b>   <b>0</b>	32, 51, 84, 92	0
All	All	411/419 (98%)	0.96	70 (17%) <b>1</b>   <b>1</b>	24, 47, 75, 92	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	THR	5.4
2	B	123	GLY	4.9
2	B	146	VAL	4.7
2	B	61	ILE	4.4
2	B	15	LEU	4.3
1	A	185	VAL	4.2
2	B	145	LEU	4.2
1	A	89	MET	4.2
1	A	192	LEU	4.1
2	B	126	LEU	3.9
1	A	228	LEU	3.9
1	A	173	LEU	3.9
1	A	171	TRP	3.8
1	A	154	LEU	3.8
2	B	143	LEU	3.8
2	B	119	LEU	3.7
1	A	235	LEU	3.6
1	A	199	TRP	3.5
1	A	135	LEU	3.5
1	A	90	ASP	3.4
1	A	234	PHE	3.3
1	A	273	LEU	3.3
2	B	120	ILE	3.3
1	A	118	THR	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	132	LEU	3.1
1	A	87	ASP	3.1
2	B	30	ILE	3.0
1	A	219	PHE	2.9
1	A	165	TYR	2.9
2	B	112	ILE	2.9
2	B	144	HIS	2.8
2	B	111	GLY	2.7
2	B	73	LEU	2.7
1	A	286	LEU	2.7
1	A	237	LEU	2.7
1	A	293	LEU	2.7
2	B	99	ILE	2.6
2	B	81	VAL	2.6
1	A	277	LEU	2.6
2	B	67	LEU	2.6
1	A	114	SER	2.5
1	A	155	MET	2.5
1	A	162	ILE	2.5
2	B	44	ILE	2.4
2	B	79	ILE	2.4
1	A	340	TYR	2.4
2	B	135	TYR	2.3
1	A	168	ILE	2.3
1	A	158	PRO	2.3
1	A	243	LEU	2.3
1	A	238	ASN	2.2
2	B	43	LEU	2.2
1	A	302	ILE	2.2
1	A	195	LEU	2.2
1	A	261	PHE	2.2
1	A	241	ILE	2.2
1	A	119	SER	2.2
2	B	56	LEU	2.1
2	B	49	GLN	2.1
2	B	50	LEU	2.1
1	A	232	VAL	2.1
2	B	40	GLN	2.1
1	A	218	LEU	2.1
1	A	269	PRO	2.1
2	B	140	GLU	2.1
1	A	172	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	121	PHE	2.1
1	A	260	LEU	2.0
1	A	200	ALA	2.0
2	B	13	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	DHA	B	76	5/6	0.97	0.17	38,40,41,42	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.