



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 01:35 PM EDT

PDB ID : 6C9U  
Title : Crystal structure of [KS3][AT3] didomain from module 3 of 6-deoxyerthronolide B synthase in complex with antibody fragment (Fab)  
Authors : Deis, L.N.; Li, X.; Mathews, I.I.; Khosla, C.  
Deposited on : 2018-01-28  
Resolution : 2.09 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.35.1

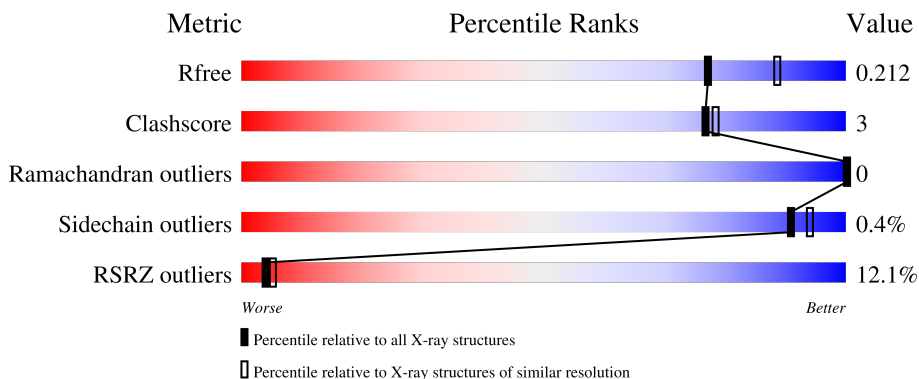
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	941	
2	L	236	
3	H	249	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 20252 atoms, of which 9690 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 6-deoxyerythronolide-B synthase EryA2, modules 3 and 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	897	13357	4175	6615	1243	1305	19	0	7	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q03132
A	2	VAL	-	expression tag	UNP Q03132
A	439	ALA	ARG	conflict	UNP Q03132
A	481	SER	THR	conflict	UNP Q03132
A	924	SER	-	expression tag	UNP Q03132
A	925	SER	-	expression tag	UNP Q03132
A	926	SER	-	expression tag	UNP Q03132
A	927	VAL	-	expression tag	UNP Q03132
A	928	ASP	-	expression tag	UNP Q03132
A	929	LYS	-	expression tag	UNP Q03132
A	930	LEU	-	expression tag	UNP Q03132
A	931	ALA	-	expression tag	UNP Q03132
A	932	ALA	-	expression tag	UNP Q03132
A	933	ALA	-	expression tag	UNP Q03132
A	934	LEU	-	expression tag	UNP Q03132
A	935	GLU	-	expression tag	UNP Q03132
A	936	HIS	-	expression tag	UNP Q03132
A	937	HIS	-	expression tag	UNP Q03132
A	938	HIS	-	expression tag	UNP Q03132
A	939	HIS	-	expression tag	UNP Q03132
A	940	HIS	-	expression tag	UNP Q03132
A	941	HIS	-	expression tag	UNP Q03132

- Molecule 2 is a protein called Light chain of Fab 1B2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	L	209	3158	1001	1562	269	320	6	0	0	0

- Molecule 3 is a protein called Heavy chain of Fab 1B2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	H	205	3052	978	1513	257	298	6	0	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		

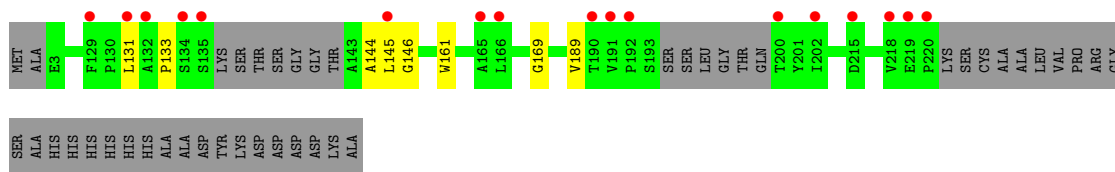
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	460	Total	O	0	2
			462	462		
6	L	81	Total	O	0	0
			81	81		
6	H	139	Total	O	0	0
			139	139		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.77Å 139.68Å 102.58Å 90.00° 97.05° 90.00°	Depositor
Resolution (Å)	46.08 – 2.09 46.08 – 2.09	Depositor EDS
% Data completeness (in resolution range)	93.9 (46.08-2.09) 93.7 (46.08-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.166 , 0.210 0.168 , 0.212	Depositor DCC
$R_{free}$ test set	2000 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtrriage
Anisotropy	0.404	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: K, CSD, NA

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	0.62	2/6867 (0.0%)	0.70	2/9332 (0.0%)
2	L	0.52	0/1630	0.65	0/2212
3	H	0.66	0/1575	0.71	0/2141
All	All	0.61	2/10072 (0.0%)	0.70	2/13685 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	VAL	CB-CG2	-5.15	1.42	1.52
1	A	592	CYS	CB-SG	5.13	1.91	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	119	ASP	CB-CG-OD1	5.61	123.34	118.30

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	6742	6615	6602	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1596	1562	1561	18	0
3	H	1539	1513	1513	5	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	462	0	0	2	0
6	H	139	0	0	0	0
6	L	81	0	0	0	0
All	All	10562	9690	9676	59	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 (59) 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:A:620:VAL:HG21	1:A:752:TYR:HE2	1.31	0.95
1:A:620:VAL:HG21	1:A:752:TYR:CE2	2.06	0.89
2:L:158:LEU:HD21	2:L:218:VAL:HG13	1.66	0.78
1:A:620:VAL:CG2	1:A:752:TYR:HE2	2.02	0.72
1:A:702:GLU:OE1	1:A:705:ARG:NH2	2.23	0.70
2:L:209:GLU:O	2:L:212:LYS:NZ	2.25	0.69
1:A:787:GLU:OE2	1:A:803:ARG:NH1	2.29	0.66
1:A:885:ASP:OD1	6:A:1101:HOH:O	2.14	0.65
2:L:158:LEU:HD11	2:L:218:VAL:HG22	1.80	0.63
1:A:679:ARG:O	1:A:682:ARG:N	2.34	0.60
1:A:157:PHE:HE1	1:A:238:VAL:HG21	1.67	0.60
2:L:158:LEU:HD11	2:L:218:VAL:CG2	2.33	0.59
2:L:146:GLN:OE1	2:L:153:SER:N	2.36	0.57
1:A:680:LEU:HB3	1:A:762:VAL:HG21	1.87	0.56
1:A:750:VAL:HG22	1:A:752:TYR:H	1.72	0.55
2:L:140:PHE:O	2:L:154:VAL:HG23	2.10	0.51
2:L:158:LEU:HD21	2:L:218:VAL:CG1	2.36	0.51
1:A:571:TRP:CH2	1:A:574:MET:HA	2.46	0.51
2:L:53:TYR:HB3	2:L:112:SER:OG	2.10	0.50
1:A:638:TRP:CZ3	1:A:872:MET:HG2	2.47	0.50
1:A:574:MET:O	1:A:608:LEU:HD22	2.13	0.49
1:A:866:SER:O	1:A:870:ARG:HG3	2.12	0.49
2:L:140:PHE:CD2	3:H:131:LEU:HB3	2.47	0.49
2:L:130:ARG:HD3	2:L:131:THR:O	2.13	0.49
1:A:597:ALA:HB3	1:A:598:PRO:HD3	1.94	0.48
2:L:158:LEU:HD23	2:L:166:ALA:HB1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ALA:O	1:A:497:GLU:HG3	2.14	0.47
2:L:185:VAL:HG12	2:L:186:THR:O	2.14	0.47
1:A:670:ALA:O	1:A:674:VAL:HG23	2.15	0.47
2:L:157:LEU:HD12	2:L:197:LEU:O	2.14	0.47
2:L:28:PRO:HB2	2:L:129:LYS:HD3	1.97	0.47
1:A:602:TRP:CZ2	1:A:622:VAL:HG12	2.50	0.47
1:A:696:GLY:O	1:A:700:VAL:HG23	2.15	0.46
1:A:748:ILE:O	1:A:750:VAL:HG12	2.15	0.46
1:A:616:GLY:O	1:A:622:VAL:HG21	2.16	0.46
1:A:677:ARG:O	1:A:681:MET:HG2	2.15	0.46
3:H:133:PRO:HD3	3:H:145:LEU:HB3	1.97	0.45
1:A:680:LEU:HD13	1:A:762:VAL:HG22	1.97	0.45
1:A:803:ARG:HG2	1:A:807:GLU:HG3	1.98	0.44
1:A:488:GLN:O	1:A:492:ILE:HG12	2.17	0.44
1:A:696:GLY:HA2	1:A:719:PRO:O	2.19	0.43
3:H:146:GLY:HA2	3:H:161:TRP:CH2	2.54	0.43
3:H:169:GLY:O	3:H:189:VAL:HA	2.18	0.43
1:A:690:MET:HB3	1:A:748:ILE:HD12	2.00	0.42
2:L:138:PHE:CD2	3:H:144:ALA:HB3	2.54	0.42
1:A:585:PHE:CD1	1:A:633:SER:HB3	2.55	0.42
2:L:219:THR:HG22	2:L:220:HIS:N	2.35	0.42
1:A:759:ILE:HG21	1:A:805:LEU:HG	2.01	0.42
1:A:2:VAL:CG1	1:A:6:GLU:HB2	2.50	0.41
1:A:755:HIS:HA	1:A:806:ARG:O	2.21	0.41
1:A:619:ARG:HB2	1:A:622:VAL:HG22	2.03	0.41
1:A:24:GLN:HG2	1:A:27[B]:ARG:NH2	2.35	0.41
1:A:689:GLY:HA3	1:A:731:LEU:HD22	2.03	0.41
1:A:27[A]:ARG:NH2	6:A:1151:HOH:O	2.53	0.41
2:L:211:HIS:O	2:L:212:LYS:HG3	2.21	0.41
1:A:162:ASP:O	1:A:910:PRO:HA	2.21	0.40
2:L:219:THR:O	2:L:220:HIS:HB2	2.21	0.40
1:A:621:ASP:HA	1:A:678:SER:HB2	2.04	0.40
1:A:309:PRO:HG2	1:A:348:ILE:HD13	2.02	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	895/941 (95%)	854 (95%)	41 (5%)	0	100	100
2	L	203/236 (86%)	189 (93%)	14 (7%)	0	100	100
3	H	199/249 (80%)	195 (98%)	4 (2%)	0	100	100
All	All	1297/1426 (91%)	1238 (96%)	59 (4%)	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	683/709 (96%)	681 (100%)	2 (0%)	92	95
2	L	185/208 (89%)	183 (99%)	2 (1%)	73	79
3	H	170/203 (84%)	170 (100%)	0	100	100
All	All	1038/1120 (93%)	1034 (100%)	4 (0%)	91	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	HIS
1	A	516	ARG
2	L	117	ARG
2	L	130	ARG

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](#)

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
1	CSD	A	203	1	3,7,8	0.84	0	1,8,10	1.49	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	CSD	A	203	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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

### 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	896/941 (95%)	0.51	103 (11%) <b>4</b> <b>6</b>	17, 36, 89, 134	0
2	L	209/236 (88%)	0.75	38 (18%) <b>1</b> <b>1</b>	23, 53, 93, 102	0
3	H	205/249 (82%)	0.28	17 (8%) <b>11</b> <b>14</b>	20, 37, 89, 110	0
All	All	1310/1426 (91%)	0.51	158 (12%) <b>4</b> <b>5</b>	17, 38, 91, 134	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	743	ILE	9.2
2	L	172	VAL	8.5
3	H	191	VAL	7.1
1	A	740	ALA	7.0
1	A	731	LEU	6.3
3	H	218	VAL	5.9
1	A	612	PRO	5.8
2	L	203	LEU	5.8
1	A	460	ARG	5.2
1	A	742	GLY	5.0
2	L	212	LYS	5.0
1	A	733	ALA	4.7
1	A	199	VAL	4.7
1	A	734	PHE	4.7
1	A	737	ASP	4.6
1	A	720	ARG	4.5
3	H	134	SER	4.5
2	L	154	VAL	4.4
1	A	418	GLY	4.2
2	L	171	LYS	4.2
2	L	151	THR	4.1
1	A	736	GLU	4.0
2	L	152	ALA	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	H	145	LEU	3.9
2	L	210	LYS	3.7
2	L	140	PHE	3.7
3	H	192	PRO	3.7
1	A	744	ARG	3.7
2	L	156	CYS	3.7
1	A	602	TRP	3.6
1	A	761	ARG	3.6
1	A	622	VAL	3.6
2	L	208	TYR	3.6
2	L	211	HIS	3.5
1	A	705	ARG	3.4
2	L	231	PHE	3.4
1	A	198	SER	3.4
1	A	212	LEU	3.4
1	A	707	TRP	3.4
2	L	209	GLU	3.4
1	A	197	ILE	3.3
1	A	152	LEU	3.3
1	A	686	GLY	3.3
1	A	732	ARG	3.3
2	L	168	VAL	3.3
1	A	154	VAL	3.3
1	A	706	PRO	3.3
1	A	597	ALA	3.2
3	H	135	SER	3.2
1	A	704	LEU	3.2
2	L	144	ASP	3.2
1	A	381	ALA	3.2
1	A	208	VAL	3.2
1	A	155	ALA	3.2
1	A	209	ALA	3.2
1	A	753	ALA	3.2
2	L	141	PRO	3.1
3	H	131	LEU	3.1
2	L	206	ALA	3.1
1	A	601	ASP	3.1
1	A	727	GLU	3.1
1	A	611	ALA	3.1
1	A	617	LEU	3.1
2	L	147	LEU	3.1
1	A	729	GLY	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	739	ALA	3.0
1	A	613	GLY	3.0
1	A	848	GLY	3.0
1	A	751	ASP	3.0
2	L	149	SER	3.0
2	L	207	ASP	3.0
2	L	224	SER	2.9
1	A	231	ALA	2.8
1	A	180	ALA	2.8
1	A	849	ALA	2.8
1	A	206	SER	2.8
1	A	151	PHE	2.8
1	A	271	THR	2.8
1	A	745	VAL	2.8
2	L	139	ILE	2.8
1	A	202	ALA	2.7
1	A	741	GLU	2.7
1	A	726	GLY	2.7
1	A	735	SER	2.7
2	L	216	CYS	2.7
3	H	190	THR	2.7
1	A	416	SER	2.7
1	A	182	ALA	2.7
1	A	752	TYR	2.7
2	L	155	VAL	2.7
1	A	201	THR	2.7
1	A	445	ILE	2.7
1	A	417	SER	2.6
2	L	204	SER	2.6
1	A	698	ALA	2.6
1	A	750	VAL	2.6
2	L	205	LYS	2.6
2	L	218	VAL	2.6
2	L	201	LEU	2.6
1	A	762	VAL	2.6
1	A	205	SER	2.6
1	A	604	VAL	2.6
1	A	861	ASP	2.6
1	A	179	PRO	2.5
1	A	730	ALA	2.5
1	A	153	GLY	2.5
1	A	1	MET	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	448	THR	2.5
2	L	148	LYS	2.5
1	A	227	VAL	2.4
2	L	217	GLU	2.4
3	H	132	ALA	2.4
3	H	202	ILE	2.4
2	L	221	GLN	2.4
1	A	226	VAL	2.4
3	H	215	ASP	2.4
1	A	738	CYS	2.4
1	A	385	VAL	2.4
1	A	687	GLU	2.4
1	A	207	LEU	2.3
1	A	758	GLN	2.3
1	A	767	LEU	2.3
1	A	232	VAL	2.3
1	A	200	ASP	2.3
1	A	229	GLY	2.3
1	A	618	ASP	2.3
1	A	684	LEU	2.2
1	A	270	VAL	2.2
3	H	219	GLU	2.2
1	A	230	ALA	2.2
1	A	619	ARG	2.2
2	L	138	PHE	2.2
3	H	129	PHE	2.2
1	A	178	ALA	2.2
1	A	382	ALA	2.2
1	A	269	GLY	2.2
1	A	615	PRO	2.2
3	H	200	THR	2.2
1	A	909	GLN	2.2
1	A	272	LEU	2.1
1	A	728	PRO	2.1
2	L	178	SER	2.1
1	A	450	ALA	2.1
2	L	142	PRO	2.1
3	H	220	PRO	2.1
1	A	383	ALA	2.1
3	H	165	ALA	2.1
1	A	228	GLY	2.1
1	A	608	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	166	LEU	2.1
1	A	567	GLN	2.1
2	L	157	LEU	2.0
2	L	191	LYS	2.0
1	A	442	ALA	2.0
1	A	183	SER	2.0
2	L	169	GLN	2.0
1	A	211	HIS	2.0
1	A	210	LEU	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
1	CSD	A	203	8/9	0.95	0.20	26,37,50,54	0

## 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<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
5	NA	A	1002	1/1	0.92	0.07	55,55,55,55	0
4	K	A	1001	1/1	0.99	0.08	37,37,37,37	0
5	NA	A	1003	1/1	0.99	0.22	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.