



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:33 pm BST

PDB ID : 6RHW
Title : Crystal structure of human CD11b I-domain (CD11b-I) in complex with Staphylococcus aureus octameric bi-component leukocidin LukGH
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Deposited on : 2019-04-23
Resolution : 2.75 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 ⓘ symbol.

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	:	2.11
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)	:	2.11

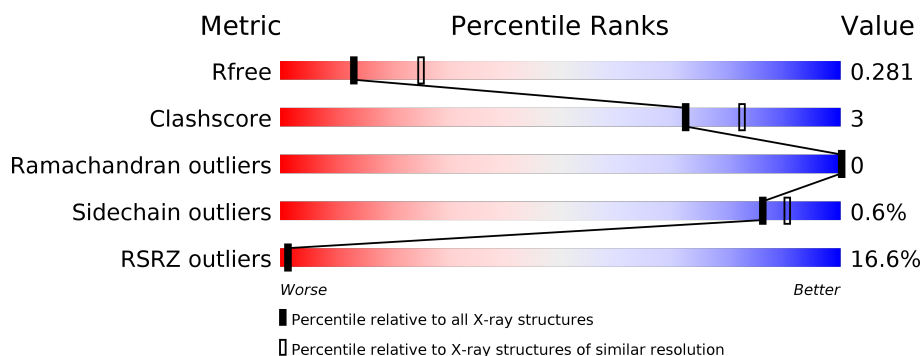
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 $\leq 5\%$. 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	G	309	<div> <div>10%</div> <div> <div>82%</div> <div>6%</div> <div>12%</div> </div> </div>
2	H	324	<div> <div>9%</div> <div> <div>78%</div> <div>6%</div> <div>16%</div> </div> </div>
3	C	195	<div> <div>31%</div> <div> <div>72%</div> <div>14%</div> <div>14%</div> </div> </div>

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
4	DMS	G	402	-	-	-	X
4	DMS	H	402	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11306 atoms, of which 5549 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-channel forming cytolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	272	Total	C	H	N	O	S	0	0	0
			4287	1378	2084	384	436	5			

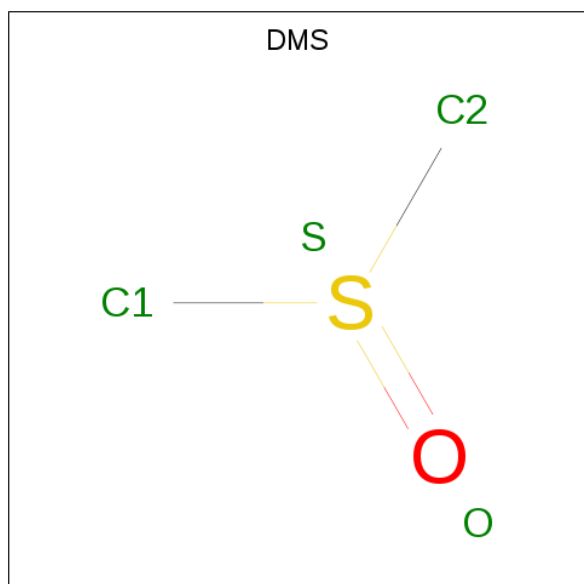
- Molecule 2 is a protein called Beta-channel forming cytolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	271	Total	C	H	N	O	0	0	0
			4322	1387	2121	379	435			

- Molecule 3 is a protein called Integrin alpha-M.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	168	Total	C	H	N	O	S	0	0	0
			2634	847	1308	227	249	3			

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
4	G	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
4	G	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
4	H	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
4	H	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
4	H	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Mg	0	0
			1	1		

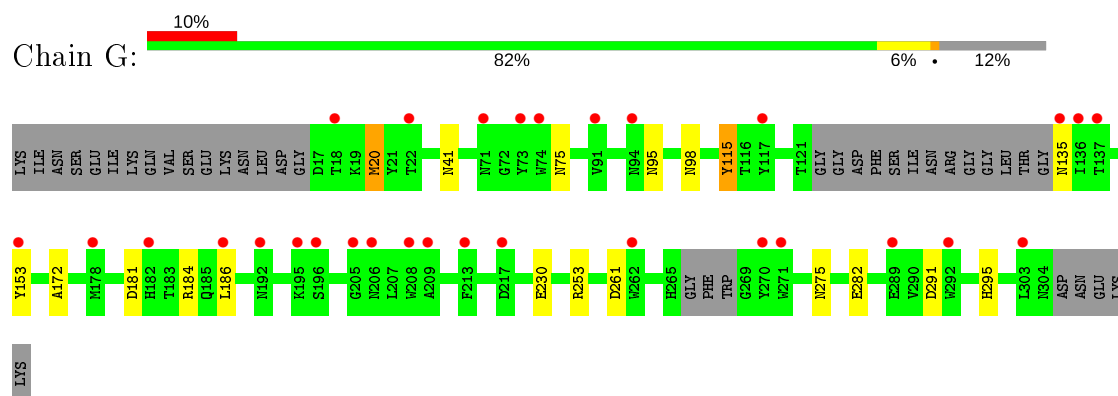
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	2	Total	O	0	0
			2	2		

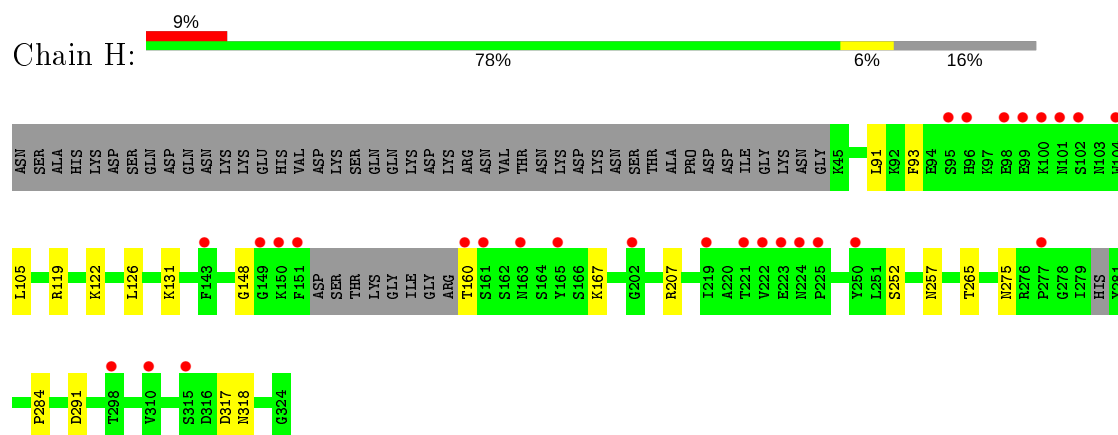
3 Residue-property plots [i](#)

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.

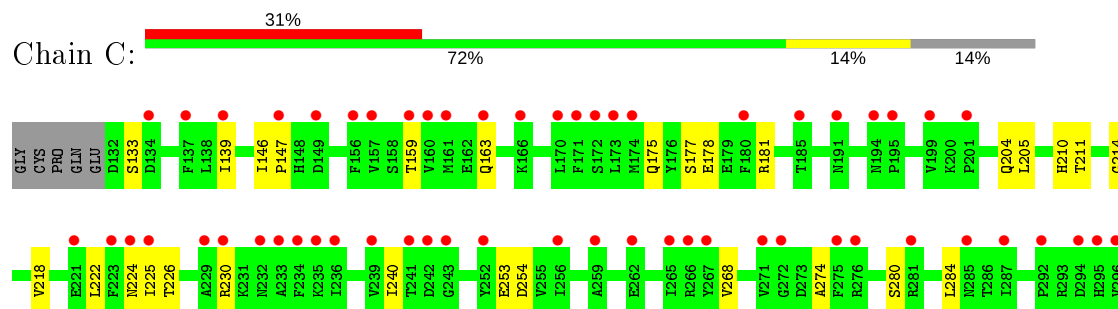
• Molecule 1: Beta-channel forming cytolsin



• Molecule 2: Beta-channel forming cytolsin



• Molecule 3: Integrin alpha-M



F297	ASN
Q298	ASN
Y299	PHE
	GLU
	ALA
	LEU
	LYS
	THR
	ILE
	GLN
	ASN
	GLN
	LEU
	ARG
	GLU
	LYS
	ILE
	PHE
	ALA
	ILE
	GLU
	GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.11Å 122.11Å 133.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.08 – 2.75 45.08 – 2.75	Depositor EDS
% Data completeness (in resolution range)	53.7 (45.08-2.75) 49.6 (45.08-2.75)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.36 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.14rc1_3177	Depositor
R, R_{free}	0.239 , 0.281 0.239 , 0.281	Depositor DCC
R_{free} test set	658 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11306	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DMS

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	G	0.26	0/2254	0.54	0/3050
2	H	0.26	0/2247	0.50	0/3037
3	C	0.26	0/1353	0.46	0/1827
All	All	0.26	0/5854	0.51	0/7914

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

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	G	2203	2084	2084	11	0
2	H	2201	2121	2120	14	0
3	C	1326	1308	1308	17	0
4	G	12	18	18	0	0
4	H	12	18	18	2	0
5	H	1	0	0	0	0
6	C	2	0	0	0	0
All	All	5757	5549	5548	38	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 (38) 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:H:148:GLY:O	2:H:160:THR:N	2.26	0.67
2:H:126:LEU:HD11	2:H:252:SER:HB3	1.78	0.66
1:G:253:ARG:NH2	1:G:282:GLU:OE1	2.32	0.62
3:C:181:ARG:HE	3:C:205:LEU:HD21	1.66	0.59
1:G:181:ASP:OD2	2:H:167:LYS:NZ	2.35	0.58
3:C:268:VAL:CG1	3:C:284:LEU:HD22	2.37	0.54
2:H:317:ASP:OD1	2:H:318:ASN:N	2.40	0.53
2:H:265:THR:HG21	4:H:402:DMS:C1	2.39	0.53
3:C:218:VAL:HG13	3:C:222:LEU:HD12	1.92	0.52
1:G:20:MET:CE	1:G:41:ASN:HB3	2.40	0.51
3:C:177:SER:OG	3:C:178:GLU:N	2.46	0.49
2:H:275:ASN:OD1	2:H:284:PRO:HB3	2.13	0.48
3:C:175:GLN:NE2	3:C:204:GLN:HA	2.29	0.48
2:H:119:ARG:CZ	3:C:253:GLU:OE2	2.62	0.48
2:H:93:PHE:CE1	2:H:105:LEU:HD13	2.49	0.48
3:C:224:ASN:ND2	3:C:226:THR:OG1	2.47	0.48
3:C:133:SER:O	3:C:230:ARG:NH2	2.48	0.47
2:H:265:THR:HG21	4:H:402:DMS:H12	1.97	0.46
3:C:175:GLN:HE22	3:C:204:GLN:HA	1.81	0.45
1:G:186:LEU:HD12	1:G:275:ASN:O	2.17	0.45
3:C:146:ILE:HG23	3:C:147:PRO:HD2	1.98	0.44
2:H:91:LEU:HD11	2:H:105:LEU:HD11	1.99	0.44
2:H:291:ASP:OD1	2:H:318:ASN:HA	2.18	0.44
3:C:211:THR:O	3:C:214:GLY:N	2.50	0.44
1:G:153:TYR:CD1	1:G:172:ALA:HA	2.53	0.43
1:G:291:ASP:O	1:G:295:HIS:N	2.52	0.43
3:C:225:ILE:HG22	3:C:225:ILE:O	2.19	0.43
1:G:95:ASN:OD1	1:G:98:ASN:ND2	2.50	0.43
3:C:178:GLU:HA	3:C:210:HIS:ND1	2.34	0.42
3:C:159:THR:O	3:C:163:GLN:N	2.51	0.42
1:G:172:ALA:HB3	1:G:184:ARG:HD2	2.02	0.42
1:G:230:GLU:OE2	2:H:131:LYS:NZ	2.52	0.42
1:G:75:ASN:HB3	1:G:261:ASP:OD1	2.20	0.41
3:C:139:ILE:HG22	3:C:240:ILE:HD12	2.03	0.41
3:C:274:ALA:O	3:C:280:SER:HB2	2.21	0.41
2:H:122:LYS:HD2	2:H:257:ASN:HB2	2.03	0.40
2:H:119:ARG:HH12	3:C:254:ASP:CG	2.25	0.40
1:G:115:TYR:O	1:G:115:TYR:HD1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	G	266/309 (86%)	254 (96%)	12 (4%)	0	100	100
2	H	265/324 (82%)	259 (98%)	6 (2%)	0	100	100
3	C	166/195 (85%)	146 (88%)	20 (12%)	0	100	100
All	All	697/828 (84%)	659 (94%)	38 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	G	246/281 (88%)	243 (99%)	3 (1%)	71	82
2	H	245/301 (81%)	244 (100%)	1 (0%)	91	93
3	C	145/173 (84%)	145 (100%)	0	100	100
All	All	636/755 (84%)	632 (99%)	4 (1%)	86	90

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

Mol	Chain	Res	Type
1	G	20	MET
1	G	115	TYR
1	G	135	ASN
2	H	207	ARG

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](#)

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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	DMS	G	401	-	3,3,3	0.64	0	3,3,3	0.45	0
4	DMS	H	403	-	3,3,3	0.66	0	3,3,3	0.53	0
4	DMS	G	403	-	3,3,3	0.66	0	3,3,3	0.57	0
4	DMS	H	401	-	3,3,3	0.67	0	3,3,3	0.55	0
4	DMS	G	402	-	3,3,3	0.66	0	3,3,3	0.47	0
4	DMS	H	402	-	3,3,3	0.67	0	3,3,3	0.66	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	402	DMS	2	0

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, 95th 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 ²)	Q<0.9
1	G	272/309 (88%)	0.94	30 (11%) 5 6	15, 48, 106, 149	0
2	H	271/324 (83%)	0.95	28 (10%) 6 7	23, 45, 112, 154	0
3	C	168/195 (86%)	1.64	60 (35%) 0 0	47, 81, 119, 135	0
All	All	711/828 (85%)	1.11	118 (16%) 1 1	15, 55, 114, 154	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	256	ILE	9.0
3	C	265	ILE	6.8
1	G	136	ILE	6.1
2	H	222	VAL	5.8
1	G	209	ALA	5.7
3	C	241	THR	5.3
2	H	102	SER	5.0
3	C	294	ASP	4.9
3	C	173	LEU	4.9
1	G	186	LEU	4.7
3	C	160	VAL	4.7
2	H	219	ILE	4.6
3	C	271	VAL	4.5
3	C	285	ASN	4.5
1	G	71	ASN	4.5
3	C	199	VAL	4.5
2	H	98	GLU	4.4
1	G	135	ASN	4.4
3	C	172	SER	4.4
1	G	74	TRP	4.4
2	H	96	HIS	4.3
1	G	205	GLY	4.3
2	H	149	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
3	C	163	GLN	4.1
2	H	160	THR	4.0
1	G	270	TYR	3.9
3	C	157	VAL	3.9
3	C	243	GLY	3.9
3	C	171	PHE	3.9
2	H	95	SER	3.8
2	H	161	SER	3.8
2	H	99	GLU	3.8
2	H	143	PHE	3.8
3	C	139	ILE	3.7
1	G	137	THR	3.7
3	C	161	MET	3.6
3	C	223	PHE	3.5
2	H	221	THR	3.4
3	C	296	VAL	3.3
2	H	163	ASN	3.2
2	H	100	LYS	3.2
3	C	239	VAL	3.2
3	C	234	PHE	3.2
3	C	225	ILE	3.1
1	G	292	TRP	3.1
3	C	275	PHE	3.1
3	C	185	THR	3.1
3	C	272	GLY	3.1
1	G	73	TYR	3.1
3	C	259	ALA	3.0
3	C	230	ARG	3.0
2	H	224	ASN	3.0
3	C	149	ASP	3.0
2	H	150	LYS	2.9
3	C	134	ASP	2.9
3	C	156	PHE	2.9
1	G	153	TYR	2.9
2	H	165	TYR	2.8
3	C	252	TYR	2.8
2	H	298	THR	2.8
3	C	191	ASN	2.8
2	H	104	TRP	2.7
3	C	281	ARG	2.7
3	C	233	ALA	2.7
1	G	217	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	267	TYR	2.7
1	G	213	PHE	2.7
2	H	223	GLU	2.7
3	C	235	LYS	2.7
1	G	196	SER	2.6
3	C	159	THR	2.6
1	G	195	LYS	2.6
1	G	262	TRP	2.6
3	C	194	ASN	2.6
1	G	18	THR	2.6
3	C	166	LYS	2.6
1	G	206	ASN	2.5
1	G	303	LEU	2.5
1	G	117	TYR	2.5
3	C	299	VAL	2.5
2	H	225	PRO	2.5
3	C	170	LEU	2.5
2	H	250	TYR	2.5
3	C	292	PRO	2.4
2	H	151	PHE	2.4
3	C	262	GLU	2.4
2	H	310	VAL	2.4
3	C	297	PHE	2.4
3	C	201	PRO	2.4
3	C	229	ALA	2.4
3	C	236	ILE	2.4
3	C	221	GLU	2.4
3	C	266	ARG	2.3
3	C	137	PHE	2.3
3	C	180	PHE	2.3
1	G	22	THR	2.3
1	G	94	ASN	2.3
1	G	208	TRP	2.3
3	C	174	MET	2.3
3	C	224	ASN	2.3
3	C	295	HIS	2.3
3	C	298	GLN	2.2
1	G	182	HIS	2.2
3	C	195	PRO	2.2
1	G	178	MET	2.2
1	G	289	GLU	2.2
3	C	232	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	276	ARG	2.2
1	G	271	TRP	2.2
2	H	315	SER	2.2
2	H	202	GLY	2.2
1	G	192	ASN	2.1
2	H	101	ASN	2.1
1	G	91	VAL	2.1
3	C	287	ILE	2.1
2	H	277	PRO	2.1
3	C	147	PRO	2.1
3	C	242	ASP	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, 95th 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 ²)	Q<0.9
4	DMS	H	402	4/4	0.73	0.47	87,105,106,106	0
4	DMS	G	402	4/4	0.76	0.49	111,134,135,135	0
4	DMS	H	403	4/4	0.84	0.44	85,104,104,104	0
4	DMS	G	403	4/4	0.88	0.33	51,62,66,66	0
4	DMS	H	401	4/4	0.92	0.29	66,80,80,80	0
4	DMS	G	401	4/4	0.94	0.33	38,46,46,46	0
5	MG	H	404	1/1	0.94	0.16	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.