



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:00 PM UTC

PDB ID : 6RHW / pdb_00006rhw
Title : Crystal structure of human CD11b I-domain (CD11b-I) in complex with Staphylococcus aureus octameric bi-component leukocidin LukGH
Authors : Trstenjak, N.; Milic, D.; Djinovic-Carugo, K.; Badarau, A.
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

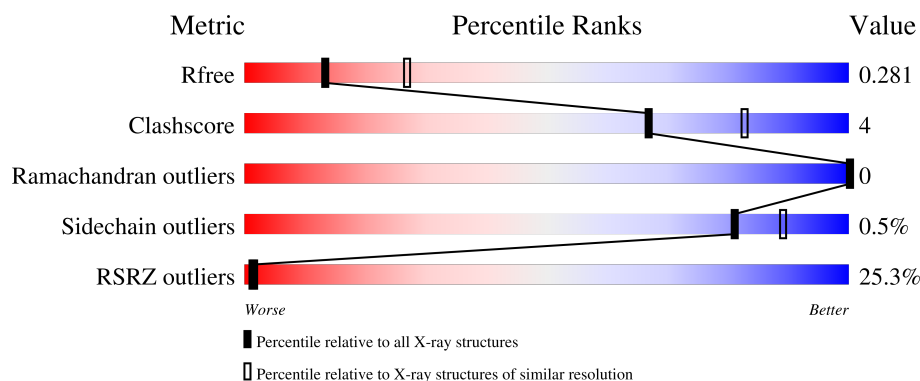
1 Overall quality at a glance

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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	21% 81% 6% 12%
2	H	324	17% 78% 6% 16%
3	C	195	31% 71% 15% 14%

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	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			

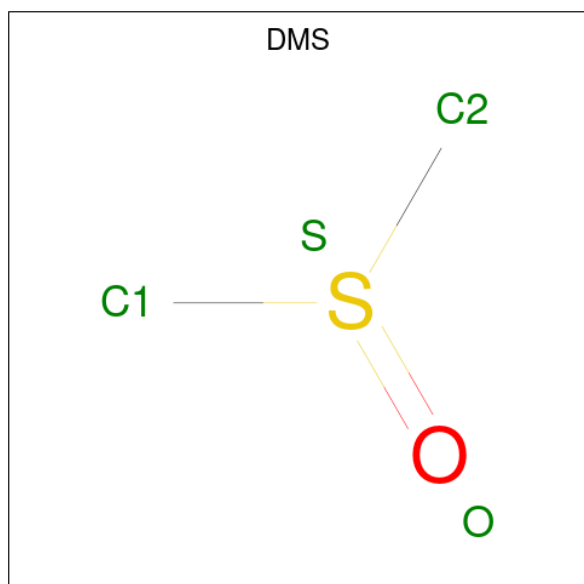
- Molecule 2 is a protein called Beta-channel forming cytolysin.

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

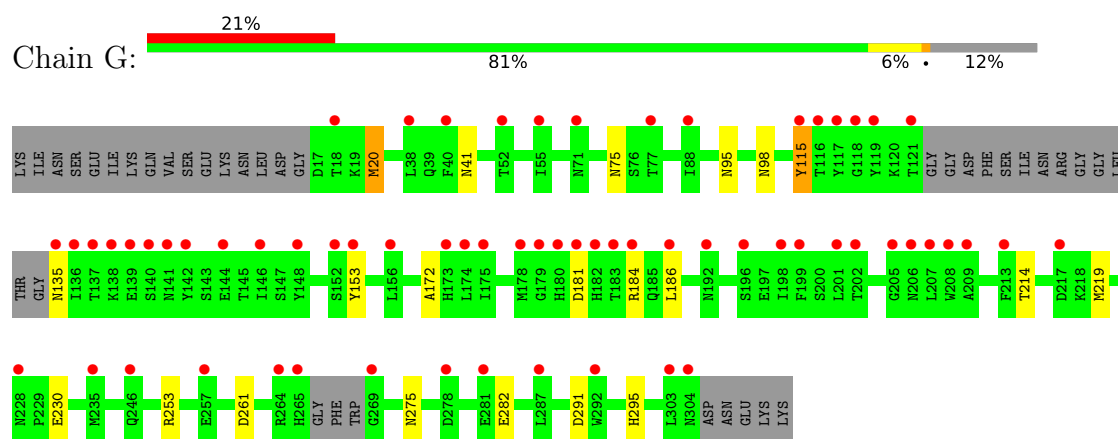
- Molecule 6 is water.

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

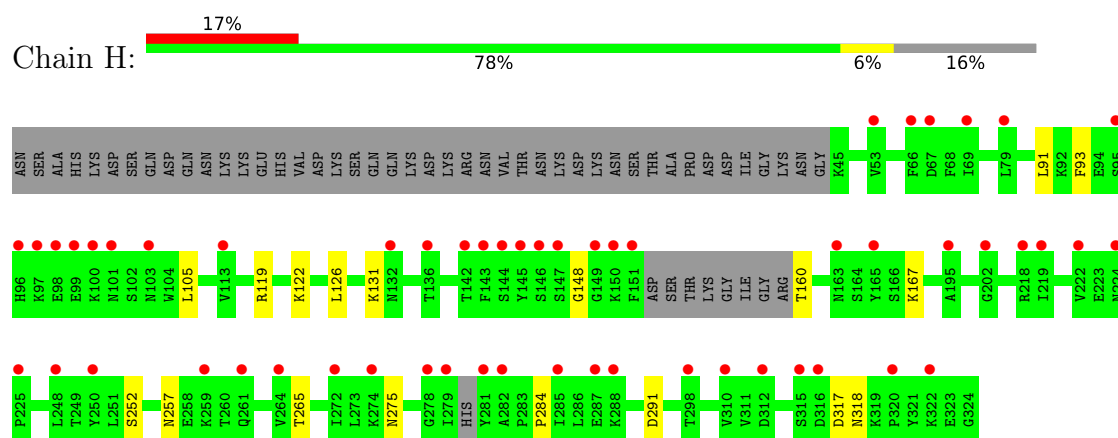
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

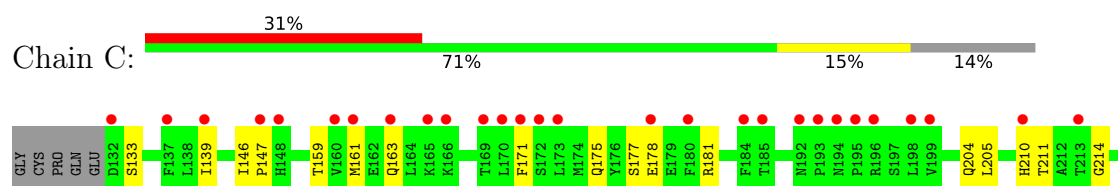
- Molecule 1: Beta-channel forming cytolsin

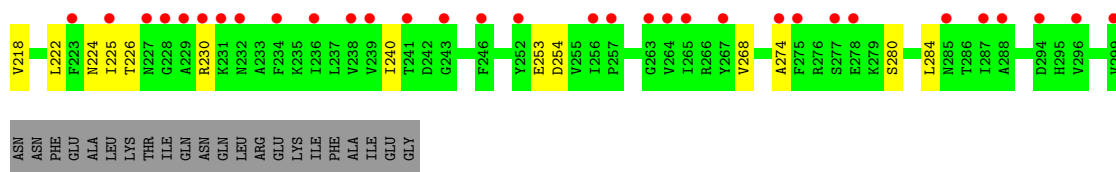


- Molecule 2: Beta-channel forming cytolsin



- Molecule 3: Integrin alpha-M





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) 49.7 (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 0.240 , 0.281	Depositor DCC
R_{free} test set	658 reflections (2.43%)	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)	0.35 , 40.1	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	0.18	0/2254	0.49	0/3050
2	H	0.17	0/2247	0.42	0/3037
3	C	0.13	0/1353	0.37	0/1827
All	All	0.16	0/5854	0.44	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	13	0
2	H	2201	2121	2120	14	0
3	C	1326	1308	1308	19	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	42	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.

All (42) 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
2:H:265:THR:HG21	4:H:402:DMS:H13	1.83	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:161:MET:HE3	3:C:171:PHE:CB	2.38	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:161:MET:HE3	3:C:171:PHE:HB2	1.92	0.50
3:C:177:SER:OG	3:C:178:GLU:N	2.46	0.49
1:G:20:MET:HE1	1:G:41:ASN:HB3	1.94	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:93:PHE:CE1	2:H:105:LEU:HD13	2.49	0.48
2:H:119:ARG:CZ	3:C:253:GLU:OE2	2.62	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:119:ARG:HH12	3:C:254:ASP:CG	2.25	0.45
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
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:225:ILE:O	3:C:225:ILE:HG22	2.19	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
1:G:214:THR:O	1:G:219:MET:HE3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:122:LYS:HD2	2:H:257:ASN:HB2	2.03	0.40
1:G:115:TYR:HD1	1:G:115:TYR:O	2.04	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	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 [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	G	246/281 (88%)	243 (99%)	3 (1%)	63	78
2	H	245/301 (81%)	245 (100%)	0	100	100
3	C	145/173 (84%)	145 (100%)	0	100	100
All	All	636/755 (84%)	633 (100%)	3 (0%)	81	89

All (3) 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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	263	ASN
2	H	88	HIS
2	H	120	ASN
2	H	244	ASN
3	C	224	ASN

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 oligosaccharides 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	402	-	3,3,3	0.67	0	3,3,3	0.49	0
4	DMS	G	403	-	3,3,3	0.67	0	3,3,3	0.59	0
4	DMS	H	403	-	3,3,3	0.67	0	3,3,3	0.55	0
4	DMS	H	401	-	3,3,3	0.68	0	3,3,3	0.57	0
4	DMS	H	402	-	3,3,3	0.68	0	3,3,3	0.68	0
4	DMS	G	401	-	3,3,3	0.65	0	3,3,3	0.47	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%)	1.35	65 (23%) 2 1	16, 54, 115, 164	0
2	H	271/324 (83%)	1.35	55 (20%) 3 2	25, 50, 122, 179	0
3	C	168/195 (86%)	1.75	60 (35%) 1 0	50, 89, 131, 156	0
All	All	711/828 (85%)	1.44	180 (25%) 1 1	16, 60, 125, 179	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	151	PHE	6.4
2	H	145	TYR	6.3
3	C	256	ILE	6.0
2	H	279	ILE	6.0
3	C	265	ILE	5.1
2	H	298	THR	4.8
3	C	228	GLY	4.8
3	C	139	ILE	4.6
1	G	153	TYR	4.4
2	H	310	VAL	4.4
2	H	163	ASN	4.3
2	H	165	TYR	4.2
2	H	224	ASN	4.2
1	G	201	LEU	4.2
2	H	248	LEU	4.2
3	C	170	LEU	4.1
2	H	143	PHE	4.1
3	C	241	THR	4.0
3	C	274	ALA	3.9
2	H	101	ASN	3.8
1	G	264	ARG	3.8
3	C	263	GLY	3.7
1	G	217	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	121	THR	3.6
1	G	202	THR	3.6
1	G	40	PHE	3.6
3	C	264	VAL	3.6
1	G	179	GLY	3.5
1	G	186	LEU	3.4
2	H	66	PHE	3.4
3	C	223	PHE	3.4
1	G	136	ILE	3.4
2	H	147	SER	3.4
3	C	173	LEU	3.4
1	G	144	GLU	3.4
1	G	137	THR	3.3
3	C	160	VAL	3.3
1	G	119	TYR	3.3
1	G	139	GLU	3.3
2	H	144	SER	3.3
3	C	277	SER	3.2
3	C	239	VAL	3.2
1	G	292	TRP	3.2
3	C	165	LYS	3.2
3	C	257	PRO	3.2
1	G	257	GLU	3.2
3	C	172	SER	3.2
2	H	150	LYS	3.1
1	G	117	TYR	3.1
1	G	88	ILE	3.1
2	H	97	LYS	3.0
2	H	281	TYR	3.0
3	C	234	PHE	3.0
1	G	38	LEU	3.0
2	H	316	ASP	3.0
3	C	137	PHE	3.0
2	H	250	TYR	3.0
1	G	55	ILE	2.9
3	C	243	GLY	2.9
1	G	246	GLN	2.9
1	G	183	THR	2.9
3	C	225	ILE	2.9
3	C	252	TYR	2.9
2	H	315	SER	2.9
1	G	269	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	209	ALA	2.9
1	G	281	GLU	2.8
3	C	299	VAL	2.8
2	H	285	ILE	2.8
1	G	278	ASP	2.8
1	G	115	TYR	2.8
1	G	213	PHE	2.8
2	H	222	VAL	2.8
2	H	272	ILE	2.7
3	C	171	PHE	2.7
3	C	231	LYS	2.7
2	H	53	VAL	2.7
2	H	132	ASN	2.7
3	C	230	ARG	2.7
2	H	264	VAL	2.7
2	H	274	LYS	2.7
1	G	142	TYR	2.7
1	G	303	LEU	2.7
2	H	202	GLY	2.7
2	H	95	SER	2.7
2	H	100	LYS	2.7
3	C	294	ASP	2.7
1	G	141	ASN	2.6
3	C	166	LYS	2.6
3	C	246	PHE	2.6
1	G	175	ILE	2.6
3	C	198	LEU	2.6
2	H	99	GLU	2.6
2	H	149	GLY	2.6
2	H	259	LYS	2.6
3	C	275	PHE	2.6
3	C	199	VAL	2.6
3	C	287	ILE	2.6
1	G	173	HIS	2.6
2	H	96	HIS	2.6
2	H	278	GLY	2.6
3	C	192	ASN	2.6
1	G	140	SER	2.5
1	G	198	ILE	2.5
3	C	180	PHE	2.5
1	G	116	THR	2.5
1	G	192	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	163	GLN	2.5
1	G	77	THR	2.5
3	C	185	THR	2.5
1	G	287	LEU	2.5
1	G	180	HIS	2.5
3	C	213	THR	2.4
3	C	278	GLU	2.4
1	G	52	THR	2.4
2	H	103	ASN	2.4
1	G	18	THR	2.4
1	G	156	LEU	2.4
2	H	69	ILE	2.4
1	G	206	ASN	2.4
3	C	148	HIS	2.4
1	G	208	TRP	2.4
1	G	178	MET	2.4
3	C	161	MET	2.4
1	G	196	SER	2.4
2	H	67	ASP	2.4
3	C	196	ARG	2.4
1	G	182	HIS	2.3
2	H	146	SER	2.3
2	H	322	LYS	2.3
1	G	138	LYS	2.3
1	G	181	ASP	2.3
1	G	207	LEU	2.3
1	G	135	ASN	2.3
1	G	205	GLY	2.3
3	C	288	ALA	2.3
2	H	98	GLU	2.3
3	C	232	ASN	2.3
2	H	219	ILE	2.2
3	C	178	GLU	2.2
1	G	71	ASN	2.2
1	G	304	ASN	2.2
3	C	147	PRO	2.2
3	C	210	HIS	2.2
3	C	194	ASN	2.2
2	H	261	GLN	2.2
2	H	136	THR	2.2
3	C	285	ASN	2.2
1	G	152	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	79	LEU	2.2
1	G	235	MET	2.2
2	H	195	ALA	2.2
2	H	225	PRO	2.2
3	C	193	PRO	2.2
3	C	132	ASP	2.2
1	G	265	HIS	2.2
3	C	184	PHE	2.2
2	H	287	GLU	2.1
1	G	184	ARG	2.1
1	G	148	TYR	2.1
3	C	267	TYR	2.1
2	H	282	ALA	2.1
1	G	199	PHE	2.1
3	C	169	THR	2.1
2	H	320	PRO	2.1
1	G	228	ASN	2.1
1	G	118	GLY	2.1
2	H	142	THR	2.1
1	G	174	LEU	2.1
3	C	236	ILE	2.1
2	H	113	VAL	2.1
3	C	296	VAL	2.1
2	H	312	ASP	2.0
2	H	288	LYS	2.0
3	C	195	PRO	2.0
3	C	227	ASN	2.0
1	G	146	ILE	2.0
3	C	229	ALA	2.0
2	H	218	ARG	2.0
3	C	238	VAL	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 oligosaccharides 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	G	402	4/4	0.72	0.25	111,134,135,135	0
4	DMS	H	402	4/4	0.75	0.41	87,105,106,106	0
4	DMS	G	403	4/4	0.84	0.20	51,62,66,66	0
4	DMS	H	401	4/4	0.89	0.25	66,80,80,80	0
4	DMS	H	403	4/4	0.89	0.37	85,104,104,104	0
4	DMS	G	401	4/4	0.90	0.14	38,46,46,46	0
5	MG	H	404	1/1	0.98	0.05	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.