



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:57 AM UTC

PDB ID : 4P1Y / pdb_00004p1y
Title : Crystal structure of staphylococcal gamma-hemolysin prepore
Authors : Yamashita, D.; Tanaka, Y.; Tanaka, I.; Yao, M.
Deposited on : 2014-02-28
Resolution : 2.99 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
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

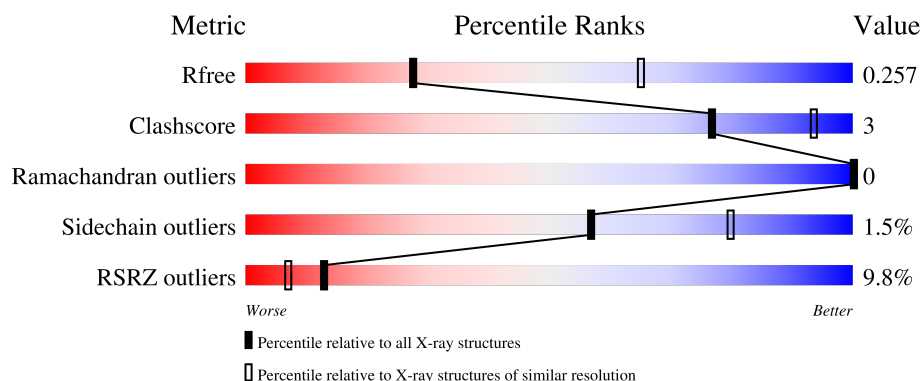
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	A	309	8% 78% 9% 14%
1	C	309	8% 77% 9% 14%
1	E	309	7% 77% 8% 14%
1	G	309	7% 79% 7% 14%
2	B	290	10% 83% 7% 9%

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Mol	Chain	Length	Quality of chain
2	D	290	10% 84% 7% 9%
2	F	290	9% 82% 9% 9%
2	H	290	9% 81% 10% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34011 atoms, of which 16788 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 Gamma-hemolysin component B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	H	N	O	S	0	0	0
			4239	1376	2070	367	422	4			
1	C	266	Total	C	H	N	O	S	0	0	0
			4227	1373	2065	366	419	4			
1	E	265	Total	C	H	N	O	S	0	0	0
			4217	1370	2060	365	418	4			
1	G	266	Total	C	H	N	O	S	0	0	0
			4228	1373	2065	366	420	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP Q931F3
A	-7	GLY	-	expression tag	UNP Q931F3
A	-6	HIS	-	expression tag	UNP Q931F3
A	-5	HIS	-	expression tag	UNP Q931F3
A	-4	HIS	-	expression tag	UNP Q931F3
A	-3	HIS	-	expression tag	UNP Q931F3
A	-2	HIS	-	expression tag	UNP Q931F3
A	-1	HIS	-	expression tag	UNP Q931F3
A	0	ALA	-	expression tag	UNP Q931F3
A	1	MET	-	expression tag	UNP Q931F3
A	177	ALA	TRP	engineered mutation	UNP Q931F3
A	198	ALA	ARG	engineered mutation	UNP Q931F3
C	-8	MET	-	expression tag	UNP Q931F3
C	-7	GLY	-	expression tag	UNP Q931F3
C	-6	HIS	-	expression tag	UNP Q931F3
C	-5	HIS	-	expression tag	UNP Q931F3
C	-4	HIS	-	expression tag	UNP Q931F3
C	-3	HIS	-	expression tag	UNP Q931F3
C	-2	HIS	-	expression tag	UNP Q931F3
C	-1	HIS	-	expression tag	UNP Q931F3
C	0	ALA	-	expression tag	UNP Q931F3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	expression tag	UNP Q931F3
C	177	ALA	TRP	engineered mutation	UNP Q931F3
C	198	ALA	ARG	engineered mutation	UNP Q931F3
E	-8	MET	-	expression tag	UNP Q931F3
E	-7	GLY	-	expression tag	UNP Q931F3
E	-6	HIS	-	expression tag	UNP Q931F3
E	-5	HIS	-	expression tag	UNP Q931F3
E	-4	HIS	-	expression tag	UNP Q931F3
E	-3	HIS	-	expression tag	UNP Q931F3
E	-2	HIS	-	expression tag	UNP Q931F3
E	-1	HIS	-	expression tag	UNP Q931F3
E	0	ALA	-	expression tag	UNP Q931F3
E	1	MET	-	expression tag	UNP Q931F3
E	177	ALA	TRP	engineered mutation	UNP Q931F3
E	198	ALA	ARG	engineered mutation	UNP Q931F3
G	-8	MET	-	expression tag	UNP Q931F3
G	-7	GLY	-	expression tag	UNP Q931F3
G	-6	HIS	-	expression tag	UNP Q931F3
G	-5	HIS	-	expression tag	UNP Q931F3
G	-4	HIS	-	expression tag	UNP Q931F3
G	-3	HIS	-	expression tag	UNP Q931F3
G	-2	HIS	-	expression tag	UNP Q931F3
G	-1	HIS	-	expression tag	UNP Q931F3
G	0	ALA	-	expression tag	UNP Q931F3
G	1	MET	-	expression tag	UNP Q931F3
G	177	ALA	TRP	engineered mutation	UNP Q931F3
G	198	ALA	ARG	engineered mutation	UNP Q931F3

- Molecule 2 is a protein called Gamma-hemolysin component A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	264	Total	C	H	N	O	S	0	0	0
			4275	1364	2132	370	406	3			
2	D	264	Total	C	H	N	O	S	0	0	0
			4275	1364	2132	370	406	3			
2	F	264	Total	C	H	N	O	S	0	0	0
			4275	1364	2132	370	406	3			
2	H	264	Total	C	H	N	O	S	0	0	0
			4275	1364	2132	370	406	3			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	expression tag	UNP P0A071
B	-8	GLY	-	expression tag	UNP P0A071
B	-7	HIS	-	expression tag	UNP P0A071
B	-6	HIS	-	expression tag	UNP P0A071
B	-5	HIS	-	expression tag	UNP P0A071
B	-4	HIS	-	expression tag	UNP P0A071
B	-3	HIS	-	expression tag	UNP P0A071
B	-2	HIS	-	expression tag	UNP P0A071
B	-1	ALA	-	expression tag	UNP P0A071
B	0	MET	-	expression tag	UNP P0A071
B	1	GLU	-	expression tag	UNP P0A071
B	2	ASN	-	expression tag	UNP P0A071
B	3	LYS	-	expression tag	UNP P0A071
B	4	ILE	-	expression tag	UNP P0A071
B	5	GLU	-	expression tag	UNP P0A071
B	6	ASP	-	expression tag	UNP P0A071
B	7	ILE	-	expression tag	UNP P0A071
B	8	GLY	-	expression tag	UNP P0A071
B	9	GLN	-	expression tag	UNP P0A071
B	10	GLY	-	expression tag	UNP P0A071
B	11	ALA	-	expression tag	UNP P0A071
B	12	GLU	-	expression tag	UNP P0A071
D	-9	MET	-	expression tag	UNP P0A071
D	-8	GLY	-	expression tag	UNP P0A071
D	-7	HIS	-	expression tag	UNP P0A071
D	-6	HIS	-	expression tag	UNP P0A071
D	-5	HIS	-	expression tag	UNP P0A071
D	-4	HIS	-	expression tag	UNP P0A071
D	-3	HIS	-	expression tag	UNP P0A071
D	-2	HIS	-	expression tag	UNP P0A071
D	-1	ALA	-	expression tag	UNP P0A071
D	0	MET	-	expression tag	UNP P0A071
D	1	GLU	-	expression tag	UNP P0A071
D	2	ASN	-	expression tag	UNP P0A071
D	3	LYS	-	expression tag	UNP P0A071
D	4	ILE	-	expression tag	UNP P0A071
D	5	GLU	-	expression tag	UNP P0A071
D	6	ASP	-	expression tag	UNP P0A071
D	7	ILE	-	expression tag	UNP P0A071
D	8	GLY	-	expression tag	UNP P0A071
D	9	GLN	-	expression tag	UNP P0A071
D	10	GLY	-	expression tag	UNP P0A071
D	11	ALA	-	expression tag	UNP P0A071

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Chain	Residue	Modelled	Actual	Comment	Reference
D	12	GLU	-	expression tag	UNP P0A071
F	-9	MET	-	expression tag	UNP P0A071
F	-8	GLY	-	expression tag	UNP P0A071
F	-7	HIS	-	expression tag	UNP P0A071
F	-6	HIS	-	expression tag	UNP P0A071
F	-5	HIS	-	expression tag	UNP P0A071
F	-4	HIS	-	expression tag	UNP P0A071
F	-3	HIS	-	expression tag	UNP P0A071
F	-2	HIS	-	expression tag	UNP P0A071
F	-1	ALA	-	expression tag	UNP P0A071
F	0	MET	-	expression tag	UNP P0A071
F	1	GLU	-	expression tag	UNP P0A071
F	2	ASN	-	expression tag	UNP P0A071
F	3	LYS	-	expression tag	UNP P0A071
F	4	ILE	-	expression tag	UNP P0A071
F	5	GLU	-	expression tag	UNP P0A071
F	6	ASP	-	expression tag	UNP P0A071
F	7	ILE	-	expression tag	UNP P0A071
F	8	GLY	-	expression tag	UNP P0A071
F	9	GLN	-	expression tag	UNP P0A071
F	10	GLY	-	expression tag	UNP P0A071
F	11	ALA	-	expression tag	UNP P0A071
F	12	GLU	-	expression tag	UNP P0A071
H	-9	MET	-	expression tag	UNP P0A071
H	-8	GLY	-	expression tag	UNP P0A071
H	-7	HIS	-	expression tag	UNP P0A071
H	-6	HIS	-	expression tag	UNP P0A071
H	-5	HIS	-	expression tag	UNP P0A071
H	-4	HIS	-	expression tag	UNP P0A071
H	-3	HIS	-	expression tag	UNP P0A071
H	-2	HIS	-	expression tag	UNP P0A071
H	-1	ALA	-	expression tag	UNP P0A071
H	0	MET	-	expression tag	UNP P0A071
H	1	GLU	-	expression tag	UNP P0A071
H	2	ASN	-	expression tag	UNP P0A071
H	3	LYS	-	expression tag	UNP P0A071
H	4	ILE	-	expression tag	UNP P0A071
H	5	GLU	-	expression tag	UNP P0A071
H	6	ASP	-	expression tag	UNP P0A071
H	7	ILE	-	expression tag	UNP P0A071
H	8	GLY	-	expression tag	UNP P0A071
H	9	GLN	-	expression tag	UNP P0A071

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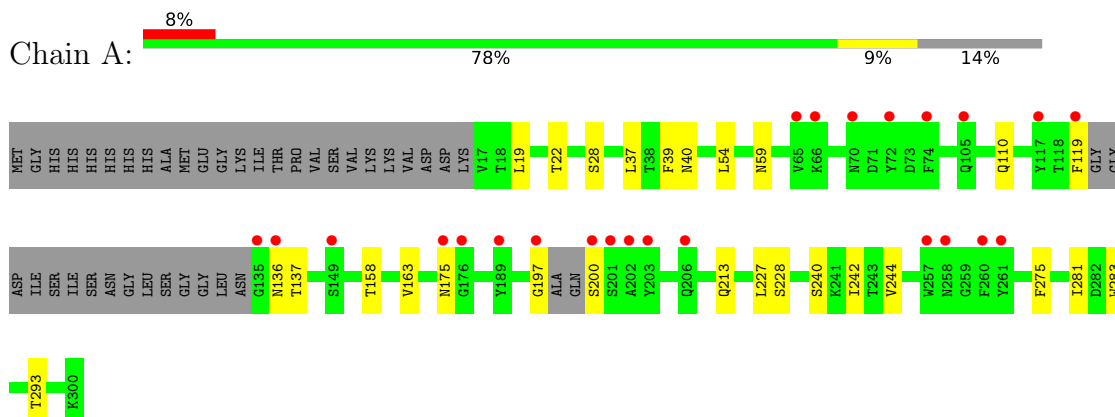
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Chain	Residue	Modelled	Actual	Comment	Reference
H	10	GLY	-	expression tag	UNP P0A071
H	11	ALA	-	expression tag	UNP P0A071
H	12	GLU	-	expression tag	UNP P0A071

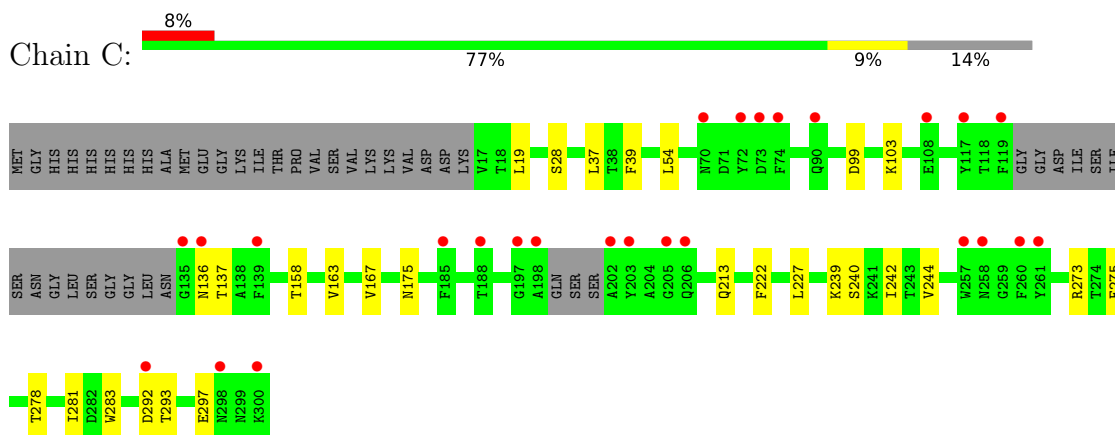
3 Residue-property plots [i](#)

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.

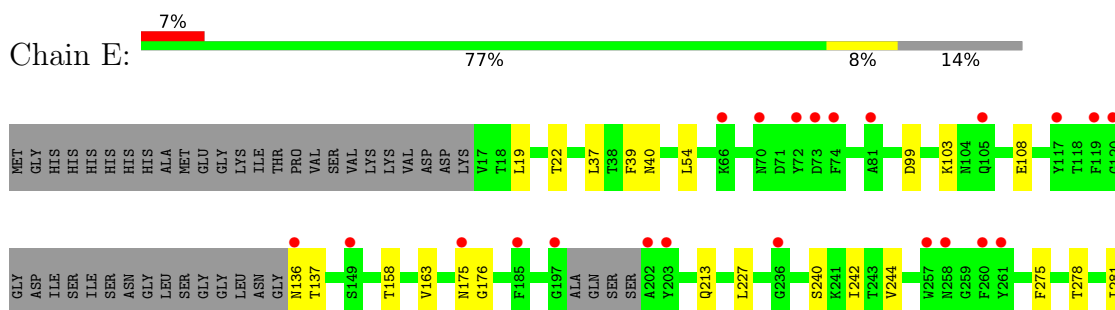
- Molecule 1: Gamma-hemolysin component B



- Molecule 1: Gamma-hemolysin component B

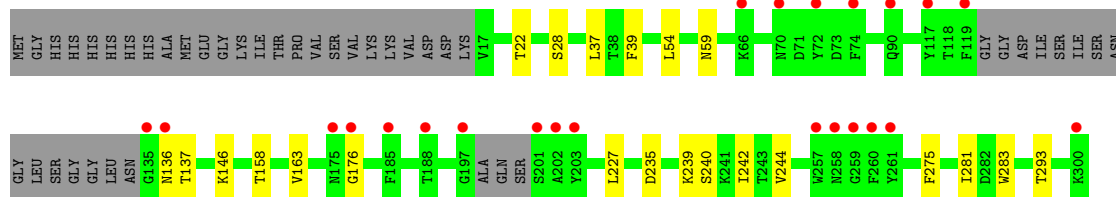
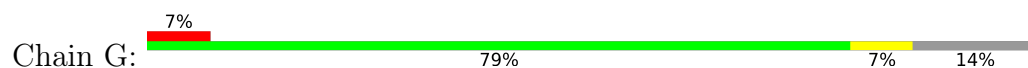


- Molecule 1: Gamma-hemolysin component B

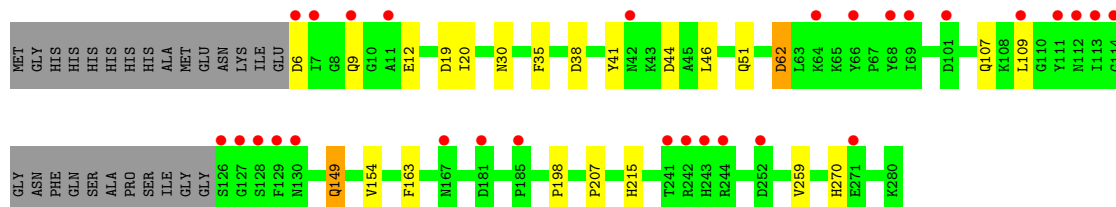
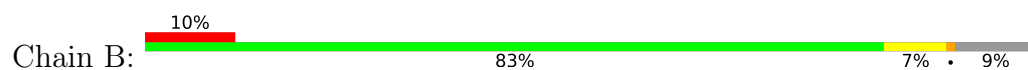




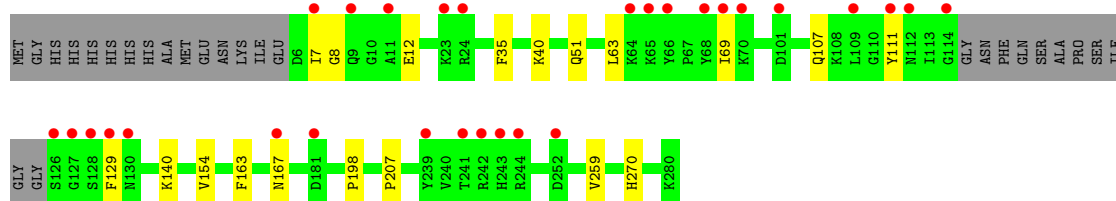
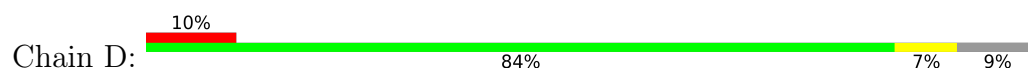
- Molecule 1: Gamma-hemolysin component B



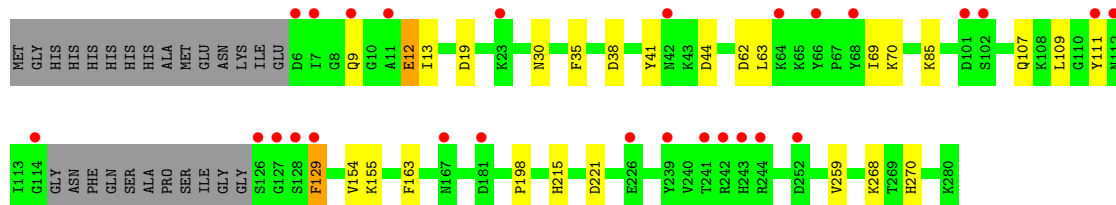
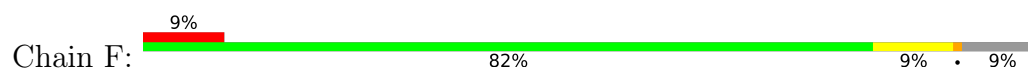
- Molecule 2: Gamma-hemolysin component A



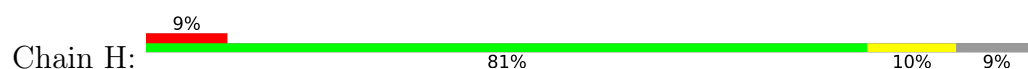
- Molecule 2: Gamma-hemolysin component A

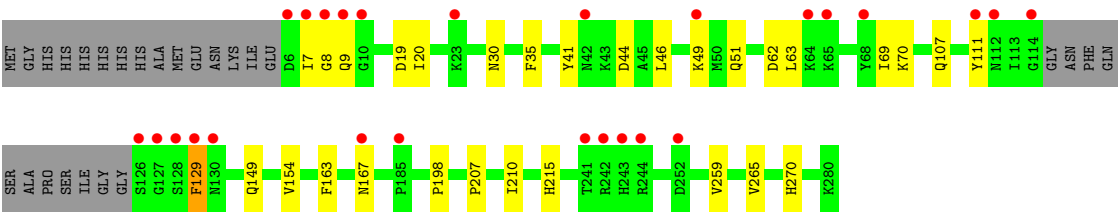


- Molecule 2: Gamma-hemolysin component A



- Molecule 2: Gamma-hemolysin component A





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.06Å 197.05Å 192.97Å 90.00° 99.04° 90.00°	Depositor
Resolution (Å)	44.40 – 2.99 44.40 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.5 (44.40-2.99) 95.5 (44.40-2.99)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.230 , 0.254 0.234 , 0.257	Depositor DCC
R_{free} test set	6970 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	1.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	34011	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.01% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/2222	0.69	0/3003
1	C	0.47	0/2215	0.70	0/2994
1	E	0.48	0/2210	0.68	1/2987 (0.0%)
1	G	0.47	0/2216	0.69	1/2995 (0.0%)
2	B	0.49	0/2191	0.80	2/2957 (0.1%)
2	D	0.49	0/2191	0.79	1/2957 (0.0%)
2	F	0.48	0/2191	0.79	1/2957 (0.0%)
2	H	0.49	0/2191	0.79	1/2957 (0.0%)
All	All	0.48	0/17627	0.74	7/23807 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	GLU	N-CA-C	6.06	118.78	110.24
1	E	176	GLY	N-CA-C	-5.99	106.32	115.66
2	B	20	ILE	N-CA-C	5.94	116.08	107.88
2	H	20	ILE	N-CA-C	5.41	115.34	107.88
2	B	12	GLU	N-CA-C	5.32	117.74	110.24
2	F	12	GLU	N-CA-C	5.31	118.04	110.24
1	G	176	GLY	N-CA-C	-5.17	107.59	115.66

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	2169	2070	2065	16	0
1	C	2162	2065	2060	17	0
1	E	2157	2060	2055	14	0
1	G	2163	2065	2060	13	0
2	B	2143	2132	2128	11	0
2	D	2143	2132	2128	10	0
2	F	2143	2132	2128	12	0
2	H	2143	2132	2128	17	0
All	All	17223	16788	16752	97	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 (97) 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:F:9:GLN:HB3	2:F:38:ASP:OD2	1.93	0.69
1:C:175:ASN:ND2	1:C:213:GLN:OE1	2.26	0.65
2:B:9:GLN:HB2	2:B:38:ASP:OD2	1.97	0.64
1:C:240:SER:HB3	1:C:283:TRP:HE1	1.68	0.58
1:C:136:ASN:OD1	1:C:137:THR:N	2.36	0.58
1:E:242:ILE:HD12	1:E:281:ILE:HD11	1.85	0.58
1:G:136:ASN:OD1	1:G:137:THR:N	2.38	0.56
1:G:240:SER:HB3	1:G:283:TRP:HE1	1.69	0.56
1:A:240:SER:HB3	1:A:283:TRP:HE1	1.69	0.56
1:A:136:ASN:OD1	1:A:137:THR:N	2.37	0.56
1:E:240:SER:HB3	1:E:283:TRP:HE1	1.71	0.55
1:A:242:ILE:HD12	1:A:281:ILE:HD11	1.91	0.53
2:B:19:ASP:OD1	2:B:30:ASN:ND2	2.38	0.53
1:G:37:LEU:HD21	1:G:244:VAL:HG21	1.91	0.53
1:A:37:LEU:HD21	1:A:244:VAL:HG21	1.90	0.52
1:E:37:LEU:HD21	1:E:244:VAL:HG21	1.90	0.52
1:C:242:ILE:HD12	1:C:281:ILE:HD11	1.91	0.52
2:F:35:PHE:CE2	2:F:270:HIS:HA	2.45	0.51
1:C:37:LEU:HD21	1:C:244:VAL:HG21	1.91	0.51
2:H:35:PHE:CE2	2:H:270:HIS:HA	2.45	0.51
2:D:35:PHE:CE2	2:D:270:HIS:HA	2.45	0.51
2:D:163:PHE:CE1	2:D:198:PRO:HG3	2.45	0.51
1:E:136:ASN:N	1:E:136:ASN:HD22	2.08	0.50
1:G:242:ILE:HD12	1:G:281:ILE:HD11	1.93	0.50
1:G:275:PHE:CE1	1:G:293:THR:HG23	2.47	0.50
2:B:35:PHE:CE2	2:B:270:HIS:HA	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD21	2:D:7:ILE:HG21	1.93	0.50
1:A:39:PHE:CE1	1:A:54:LEU:HD13	2.46	0.49
2:B:62:ASP:OD2	2:B:62:ASP:N	2.45	0.49
2:B:163:PHE:CE1	2:B:198:PRO:HG3	2.47	0.48
1:A:275:PHE:CE1	1:A:293:THR:HG23	2.48	0.48
1:C:39:PHE:CE1	1:C:54:LEU:HD13	2.49	0.48
1:C:275:PHE:CE1	1:C:293:THR:HG23	2.48	0.48
2:H:111:TYR:CE1	2:H:129:PHE:HB2	2.49	0.48
2:F:19:ASP:OD1	2:F:30:ASN:ND2	2.40	0.48
2:B:109:LEU:HD11	2:H:167:ASN:HA	1.96	0.47
2:F:163:PHE:CE1	2:F:198:PRO:HG3	2.49	0.47
2:H:163:PHE:CE1	2:H:198:PRO:HG3	2.50	0.47
1:E:275:PHE:CE1	1:E:293:THR:HG23	2.50	0.47
2:D:63:LEU:HD12	2:D:69:ILE:HB	1.98	0.46
1:G:59:ASN:HB2	2:H:149:GLN:HG3	1.98	0.46
1:G:39:PHE:CE1	1:G:54:LEU:HD13	2.51	0.46
2:F:62:ASP:OD1	2:F:70:LYS:HE3	2.16	0.46
1:E:175:ASN:ND2	1:E:213:GLN:OE1	2.47	0.45
2:B:35:PHE:CD1	2:B:46:LEU:HD13	2.52	0.45
2:H:62:ASP:OD1	2:H:70:LYS:HE3	2.16	0.45
1:E:39:PHE:CE1	1:E:54:LEU:HD13	2.52	0.44
1:C:28:SER:HB2	1:C:275:PHE:CD1	2.53	0.44
2:F:111:TYR:CE1	2:F:129:PHE:HB2	2.52	0.44
1:E:19:LEU:HD11	1:E:40:ASN:HB3	2.00	0.44
2:F:44:ASP:HB2	2:F:215:HIS:HB3	2.00	0.44
1:E:158:THR:HG23	1:E:163:VAL:HA	1.99	0.44
2:B:51:GLN:HA	2:B:207:PRO:O	2.18	0.43
2:H:19:ASP:OD1	2:H:30:ASN:ND2	2.44	0.43
1:A:119:PHE:HB3	2:H:129:PHE:CE2	2.52	0.43
2:H:35:PHE:CD1	2:H:46:LEU:HD13	2.54	0.43
1:G:239:LYS:HA	1:G:281:ILE:O	2.19	0.43
1:A:59:ASN:HB2	2:B:149:GLN:HG3	2.01	0.43
1:A:119:PHE:HB3	2:H:129:PHE:HE2	1.84	0.43
2:D:7:ILE:HG23	2:D:8:GLY:N	2.33	0.42
2:D:140:LYS:HE3	1:E:108:GLU:OE2	2.19	0.42
1:E:22:THR:HA	2:F:41:TYR:CE1	2.54	0.42
2:H:49:LYS:HD2	2:H:210:ILE:HG12	2.01	0.42
1:A:28:SER:HB2	1:A:275:PHE:CD1	2.54	0.42
1:C:19:LEU:HD23	2:D:40:LYS:HD2	2.02	0.42
1:A:19:LEU:HD11	1:A:40:ASN:HB3	2.01	0.42
1:C:278:THR:HB	1:C:292:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:THR:HA	2:F:41:TYR:HE1	1.85	0.42
1:G:158:THR:HG23	1:G:163:VAL:HA	2.01	0.42
1:A:22:THR:HA	2:B:41:TYR:CE1	2.55	0.42
1:C:37:LEU:HB3	1:C:39:PHE:CE2	2.55	0.42
1:G:22:THR:HA	2:H:41:TYR:CE1	2.55	0.42
1:A:158:THR:HG23	1:A:163:VAL:HA	2.02	0.42
1:A:175:ASN:ND2	1:A:213:GLN:OE1	2.50	0.42
1:A:110:GLN:OE1	1:A:110:GLN:N	2.53	0.42
1:E:99:ASP:OD1	1:E:103:LYS:NZ	2.52	0.41
2:F:63:LEU:HD12	2:F:69:ILE:HB	2.02	0.41
2:B:44:ASP:HB2	2:B:215:HIS:HB3	2.01	0.41
1:C:239:LYS:HA	1:C:281:ILE:O	2.20	0.41
1:A:197:GLY:O	1:A:200:SER:N	2.54	0.41
1:C:99:ASP:OD1	1:C:103:LYS:NZ	2.49	0.41
1:G:235:ASP:OD1	1:G:235:ASP:N	2.50	0.41
2:D:167:ASN:HA	2:F:109:LEU:HD11	2.03	0.41
1:C:273:ARG:CZ	1:C:297:GLU:HG3	2.50	0.41
2:H:35:PHE:HZ	2:H:265:VAL:HG13	1.86	0.41
1:C:158:THR:HG23	1:C:163:VAL:HA	2.01	0.41
1:E:278:THR:HB	1:E:292:ASP:HB2	2.03	0.41
2:H:8:GLY:HA2	2:H:9:GLN:HA	1.92	0.41
2:H:51:GLN:HA	2:H:207:PRO:O	2.21	0.41
2:H:63:LEU:HD12	2:H:69:ILE:HB	2.03	0.41
2:F:221:ASP:OD2	2:F:268:LYS:HE2	2.20	0.40
1:C:167:VAL:HG21	1:C:222:PHE:CZ	2.56	0.40
2:D:51:GLN:HA	2:D:207:PRO:O	2.22	0.40
2:D:111:TYR:CE1	2:D:129:PHE:HB2	2.56	0.40
2:H:44:ASP:HB2	2:H:215:HIS:HB3	2.02	0.40
1:G:37:LEU:HB3	1:G:39:PHE:CE2	2.56	0.40
1:G:28:SER:HB2	1:G:275:PHE:CD1	2.56	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	A	261/309 (84%)	255 (98%)	6 (2%)	0	100	100
1	C	260/309 (84%)	252 (97%)	8 (3%)	0	100	100
1	E	259/309 (84%)	252 (97%)	7 (3%)	0	100	100
1	G	260/309 (84%)	254 (98%)	6 (2%)	0	100	100
2	B	260/290 (90%)	252 (97%)	8 (3%)	0	100	100
2	D	260/290 (90%)	252 (97%)	8 (3%)	0	100	100
2	F	260/290 (90%)	251 (96%)	9 (4%)	0	100	100
2	H	260/290 (90%)	254 (98%)	6 (2%)	0	100	100
All	All	2080/2396 (87%)	2022 (97%)	58 (3%)	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	A	236/269 (88%)	234 (99%)	2 (1%)	73	86
1	C	234/269 (87%)	233 (100%)	1 (0%)	84	90
1	E	234/269 (87%)	232 (99%)	2 (1%)	70	85
1	G	235/269 (87%)	233 (99%)	2 (1%)	70	85
2	B	237/257 (92%)	231 (98%)	6 (2%)	42	72
2	D	237/257 (92%)	234 (99%)	3 (1%)	61	81
2	F	237/257 (92%)	229 (97%)	8 (3%)	32	66
2	H	237/257 (92%)	232 (98%)	5 (2%)	47	75
All	All	1887/2104 (90%)	1858 (98%)	29 (2%)	57	80

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	LEU
1	A	228	SER
2	B	6	ASP
2	B	62	ASP
2	B	107	GLN
2	B	149	GLN
2	B	154	VAL
2	B	259	VAL
1	C	227	LEU
2	D	107	GLN
2	D	154	VAL
2	D	259	VAL
1	E	137	THR
1	E	227	LEU
2	F	12	GLU
2	F	13	ILE
2	F	85	LYS
2	F	107	GLN
2	F	129	PHE
2	F	154	VAL
2	F	155	LYS
2	F	259	VAL
1	G	146	LYS
1	G	227	LEU
2	H	7	ILE
2	H	107	GLN
2	H	129	PHE
2	H	154	VAL
2	H	259	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	113	ASN
1	A	298	ASN
2	B	130	ASN
2	B	215	HIS
1	C	61	ASN
1	C	90	GLN
1	C	286	HIS
1	C	298	ASN
2	D	112	ASN

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Mol	Chain	Res	Type
2	D	180	GLN
2	D	215	HIS
1	E	90	GLN
1	E	113	ASN
2	F	130	ASN
2	F	138	ASN
2	F	161	ASN
1	G	90	GLN
1	G	113	ASN
1	G	144	ASN
1	G	147	GLN
1	G	212	HIS
1	G	298	ASN
2	H	215	HIS

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](#)

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, 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	A	267/309 (86%)	0.65	24 (8%)	15 8	16, 49, 109, 152	0
1	C	266/309 (86%)	0.68	26 (9%)	13 7	18, 50, 109, 142	0
1	E	265/309 (85%)	0.61	23 (8%)	16 8	16, 49, 102, 136	0
1	G	266/309 (86%)	0.64	23 (8%)	16 8	17, 49, 109, 146	0
2	B	264/290 (91%)	0.69	29 (10%)	10 6	19, 51, 109, 165	0
2	D	264/290 (91%)	0.68	29 (10%)	10 6	19, 50, 109, 175	0
2	F	264/290 (91%)	0.70	27 (10%)	12 6	21, 50, 99, 174	0
2	H	264/290 (91%)	0.64	26 (9%)	13 7	18, 50, 101, 176	0
All	All	2120/2396 (88%)	0.66	207 (9%)	13 7	16, 50, 109, 176	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	119	PHE	10.6
1	G	119	PHE	10.1
1	A	119	PHE	9.4
1	E	119	PHE	8.8
1	A	197	GLY	8.1
1	E	120	GLY	7.7
1	G	197	GLY	7.6
1	E	202	ALA	7.0
2	F	243	HIS	6.9
1	C	202	ALA	6.7
1	G	201	SER	6.7
2	B	114	GLY	6.7
1	C	198	ALA	6.4
1	E	197	GLY	6.4
1	G	202	ALA	6.2
2	D	111	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
2	D	114	GLY	6.0
1	A	117	TYR	6.0
2	H	243	HIS	6.0
2	B	243	HIS	5.9
2	H	126	SER	5.8
2	B	111	TYR	5.7
2	B	126	SER	5.6
2	F	7	ILE	5.5
2	H	114	GLY	5.5
1	C	117	TYR	5.4
2	D	243	HIS	5.3
1	A	202	ALA	5.2
2	F	126	SER	5.2
2	B	127	GLY	5.2
1	G	117	TYR	5.1
1	A	260	PHE	4.9
1	G	135	GLY	4.9
1	C	261	TYR	4.9
1	C	135	GLY	4.9
2	H	111	TYR	4.9
2	B	129	PHE	4.8
2	D	129	PHE	4.8
1	E	117	TYR	4.8
2	B	128	SER	4.7
2	F	114	GLY	4.7
2	H	127	GLY	4.7
2	F	111	TYR	4.7
2	H	129	PHE	4.6
1	A	201	SER	4.5
1	A	200	SER	4.5
2	H	128	SER	4.5
1	C	260	PHE	4.4
1	G	260	PHE	4.4
1	E	261	TYR	4.4
2	D	167	ASN	4.4
2	D	68	TYR	4.4
1	E	260	PHE	4.3
2	F	127	GLY	4.3
2	D	127	GLY	4.3
2	B	7	ILE	4.2
2	D	112	ASN	4.2
1	G	261	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	112	ASN	4.1
2	F	64	LYS	4.0
1	C	197	GLY	4.0
1	G	258	ASN	3.9
2	H	9	GLN	3.9
2	H	64	LYS	3.9
2	F	128	SER	3.8
1	C	206	GLN	3.8
1	A	258	ASN	3.8
1	E	74	PHE	3.6
1	A	135	GLY	3.6
1	E	258	ASN	3.6
2	D	64	LYS	3.5
2	F	112	ASN	3.5
2	B	68	TYR	3.4
2	B	64	LYS	3.4
2	D	126	SER	3.4
1	G	136	ASN	3.4
1	C	203	TYR	3.4
1	C	70	ASN	3.4
1	A	136	ASN	3.3
1	A	261	TYR	3.3
2	H	7	ILE	3.3
2	B	9	GLN	3.3
2	D	7	ILE	3.2
2	F	11	ALA	3.2
2	F	167	ASN	3.1
2	D	128	SER	3.1
1	A	74	PHE	3.1
2	F	68	TYR	3.0
1	C	90	GLN	3.0
2	B	42	ASN	3.0
2	F	9	GLN	3.0
2	D	181	ASP	3.0
2	F	129	PHE	3.0
2	H	241	THR	2.9
2	D	244	ARG	2.9
1	E	72	TYR	2.9
1	C	188	THR	2.9
2	D	70	LYS	2.9
2	H	23	LYS	2.9
1	G	72	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	74	PHE	2.9
1	E	203	TYR	2.9
1	A	257	TRP	2.8
1	A	70	ASN	2.8
2	D	69	ILE	2.8
2	D	65	LYS	2.8
2	H	68	TYR	2.8
2	F	23	LYS	2.8
2	H	242	ARG	2.7
2	H	112	ASN	2.7
2	F	241	THR	2.7
2	F	181	ASP	2.7
2	D	242	ARG	2.7
1	G	203	TYR	2.7
2	H	167	ASN	2.7
2	B	181	ASP	2.7
2	D	239	TYR	2.7
2	D	66	TYR	2.6
2	B	252	ASP	2.6
2	F	101	ASP	2.6
2	B	11	ALA	2.6
2	F	252	ASP	2.6
1	E	149	SER	2.6
1	E	66	LYS	2.6
2	H	252	ASP	2.6
2	H	65	LYS	2.6
2	H	42	ASN	2.6
2	B	6	ASP	2.6
2	B	101	ASP	2.6
1	G	257	TRP	2.5
1	C	185	PHE	2.5
1	C	136	ASN	2.5
2	D	101	ASP	2.5
2	F	226	GLU	2.5
2	F	242	ARG	2.5
1	C	258	ASN	2.5
2	B	130	ASN	2.5
1	C	300	LYS	2.4
1	G	74	PHE	2.4
1	A	203	TYR	2.4
1	G	176	GLY	2.4
1	A	105	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	109	LEU	2.4
2	D	252	ASP	2.4
1	A	149	SER	2.4
1	A	206	GLN	2.4
1	E	70	ASN	2.3
1	C	73	ASP	2.3
2	D	11	ALA	2.3
1	C	108	GLU	2.3
2	F	6	ASP	2.3
2	H	49	LYS	2.3
1	G	70	ASN	2.3
1	G	175	ASN	2.3
2	H	130	ASN	2.3
1	C	292	ASP	2.3
1	G	300	LYS	2.3
2	D	23	LYS	2.3
1	C	257	TRP	2.3
1	C	205	GLY	2.3
1	E	81	ALA	2.2
2	D	130	ASN	2.2
2	B	244	ARG	2.2
1	G	188	THR	2.2
2	B	241	THR	2.2
2	D	241	THR	2.2
2	B	271	GLU	2.2
2	B	167	ASN	2.2
1	E	105	GLN	2.2
2	D	9	GLN	2.2
1	E	292	ASP	2.2
1	C	72	TYR	2.2
1	E	236	GLY	2.2
2	H	8	GLY	2.2
1	C	139	PHE	2.2
1	C	298	ASN	2.2
1	E	136	ASN	2.2
2	B	113	ILE	2.2
1	G	66	LYS	2.2
1	A	175	ASN	2.2
1	A	65	VAL	2.2
2	F	244	ARG	2.1
1	E	73	ASP	2.1
1	G	259	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	102	SER	2.1
1	G	90	GLN	2.1
2	D	109	LEU	2.1
2	F	66	TYR	2.1
1	E	175	ASN	2.1
2	F	42	ASN	2.1
2	H	185	PRO	2.1
1	G	185	PHE	2.1
2	H	6	ASP	2.1
2	D	24	ARG	2.1
2	H	244	ARG	2.1
1	A	72	TYR	2.1
1	A	189	TYR	2.1
1	A	66	LYS	2.0
1	A	176	GLY	2.0
1	E	185	PHE	2.0
1	E	257	TRP	2.0
2	B	185	PRO	2.0
2	B	242	ARG	2.0
2	H	10	GLY	2.0
2	B	69	ILE	2.0
2	B	66	TYR	2.0
2	F	239	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.