



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:10 PM BST

PDB ID : 4P1X  
Title : Crystal structure of staphylococcal LUK prepore  
Authors : Yamashita, D.; Tanaka, Y.; Tanaka, I.; Yao, M.  
Deposited on : 2014-02-28  
Resolution : 2.40 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

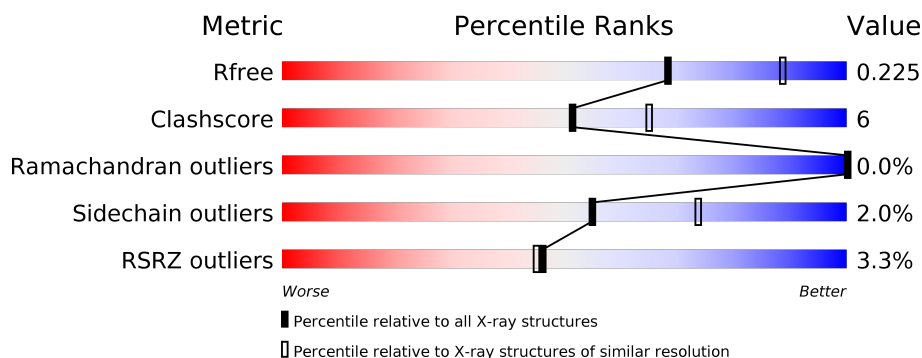
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	B	296	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	296	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div></div> <div>13%</div> </div> </div>
1	F	296	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>10%</div> <div>•</div> <div>14%</div> </div> </div>
1	H	296	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
2	A	309	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div></div> <div>14%</div> </div> </div>
2	C	309	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>10%</div> <div>•</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	E	309	<div><div></div><div>2%</div><div>80%</div><div>6%</div><div>14%</div></div>
2	G	309	<div><div></div><div>4%</div><div>77%</div><div>9%</div><div>14%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34827 atoms, of which 16598 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 C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	257	Total	C	H	N	O	S	0	0	0
			4156	1337	2050	361	405	3			
1	D	257	Total	C	H	N	O	S	0	0	0
			4156	1337	2050	361	405	3			
1	F	255	Total	C	H	N	O	S	0	0	0
			4119	1326	2033	356	401	3			
1	H	258	Total	C	H	N	O	S	0	0	0
			4163	1339	2053	362	406	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	expression tag	UNP Q99RL1
B	-10	GLY	-	expression tag	UNP Q99RL1
B	-9	HIS	-	expression tag	UNP Q99RL1
B	-8	HIS	-	expression tag	UNP Q99RL1
B	-7	HIS	-	expression tag	UNP Q99RL1
B	-6	HIS	-	expression tag	UNP Q99RL1
B	-5	HIS	-	expression tag	UNP Q99RL1
B	-4	HIS	-	expression tag	UNP Q99RL1
B	-3	ALA	-	expression tag	UNP Q99RL1
B	-2	MET	-	expression tag	UNP Q99RL1
D	-11	MET	-	expression tag	UNP Q99RL1
D	-10	GLY	-	expression tag	UNP Q99RL1
D	-9	HIS	-	expression tag	UNP Q99RL1
D	-8	HIS	-	expression tag	UNP Q99RL1
D	-7	HIS	-	expression tag	UNP Q99RL1
D	-6	HIS	-	expression tag	UNP Q99RL1
D	-5	HIS	-	expression tag	UNP Q99RL1
D	-4	HIS	-	expression tag	UNP Q99RL1
D	-3	ALA	-	expression tag	UNP Q99RL1
D	-2	MET	-	expression tag	UNP Q99RL1
F	-11	MET	-	expression tag	UNP Q99RL1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	GLY	-	expression tag	UNP Q99RL1
F	-9	HIS	-	expression tag	UNP Q99RL1
F	-8	HIS	-	expression tag	UNP Q99RL1
F	-7	HIS	-	expression tag	UNP Q99RL1
F	-6	HIS	-	expression tag	UNP Q99RL1
F	-5	HIS	-	expression tag	UNP Q99RL1
F	-4	HIS	-	expression tag	UNP Q99RL1
F	-3	ALA	-	expression tag	UNP Q99RL1
F	-2	MET	-	expression tag	UNP Q99RL1
H	-11	MET	-	expression tag	UNP Q99RL1
H	-10	GLY	-	expression tag	UNP Q99RL1
H	-9	HIS	-	expression tag	UNP Q99RL1
H	-8	HIS	-	expression tag	UNP Q99RL1
H	-7	HIS	-	expression tag	UNP Q99RL1
H	-6	HIS	-	expression tag	UNP Q99RL1
H	-5	HIS	-	expression tag	UNP Q99RL1
H	-4	HIS	-	expression tag	UNP Q99RL1
H	-3	ALA	-	expression tag	UNP Q99RL1
H	-2	MET	-	expression tag	UNP Q99RL1

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	265	Total	C	H	N	O	S	0	0	0
			4259	1381	2083	372	420	3			
2	C	267	Total	C	H	N	O	S	0	0	0
			4281	1387	2093	375	423	3			
2	E	267	Total	C	H	N	O	S	0	0	0
			4281	1387	2093	375	423	3			
2	G	266	Total	C	H	N	O	S	0	0	0
			4267	1383	2087	373	421	3			

There are 44 discrepancies between the modelled and reference sequences:

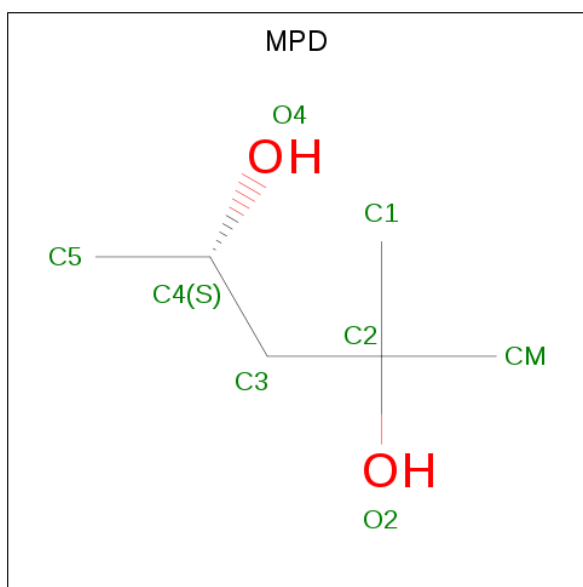
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP Q931F3
A	-7	GLY	-	expression tag	UNP Q931F3
A	-6	HIS	-	expression tag	UNP Q931F3
A	-5	HIS	-	expression tag	UNP Q931F3
A	-4	HIS	-	expression tag	UNP Q931F3
A	-3	HIS	-	expression tag	UNP Q931F3
A	-2	HIS	-	expression tag	UNP Q931F3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP Q931F3
A	0	ALA	-	expression tag	UNP Q931F3
A	1	MET	-	expression tag	UNP Q931F3
A	256	ARG	CYS	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
C	1	MET	-	expression tag	UNP Q931F3
C	256	ARG	CYS	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	256	ARG	CYS	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	256	ARG	CYS	engineered mutation	UNP Q931F3

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	C	1	Total	C	H	O	0	0
			22	6	14	2		
3	E	1	Total	C	H	O	0	0
			22	6	14	2		
3	G	1	Total	C	H	O	0	0
			22	6	14	2		

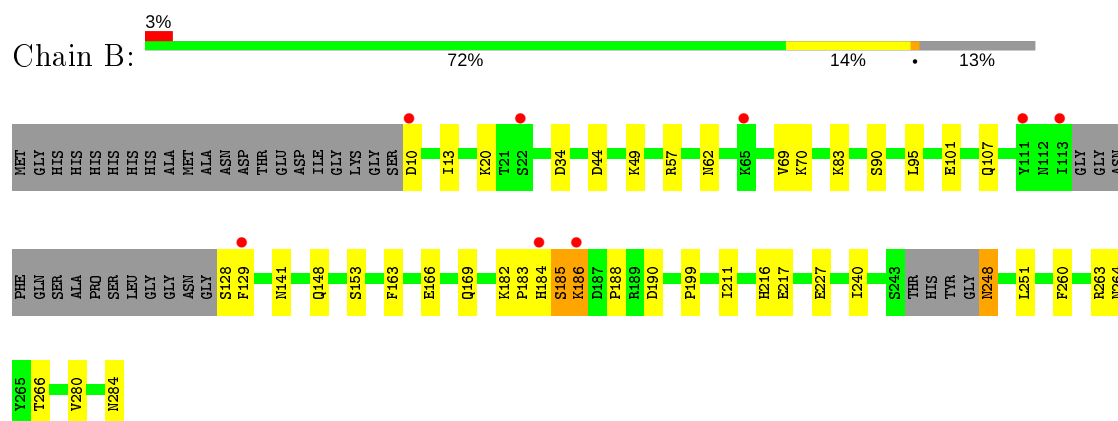
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	140	Total	O	0	0
			140	140		
4	A	120	Total	O	0	0
			120	120		
4	C	122	Total	O	0	0
			122	122		
4	D	141	Total	O	0	0
			141	141		
4	E	118	Total	O	0	0
			118	118		
4	F	151	Total	O	0	0
			151	151		
4	G	117	Total	O	0	0
			117	117		
4	H	148	Total	O	0	0
			148	148		

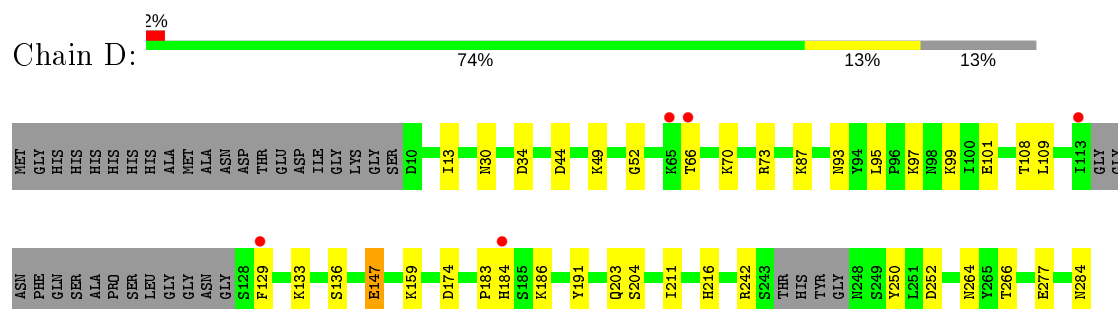
### 3 Residue-property plots [i](#)

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.

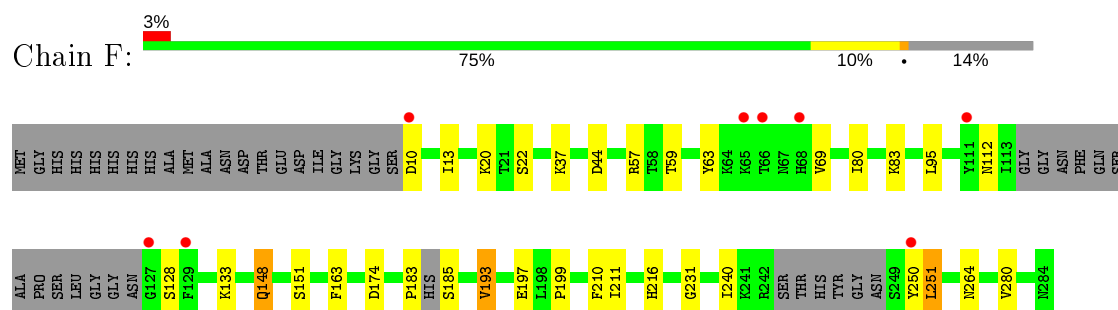
- Molecule 1: Gamma-hemolysin component C



- Molecule 1: Gamma-hemolysin component C

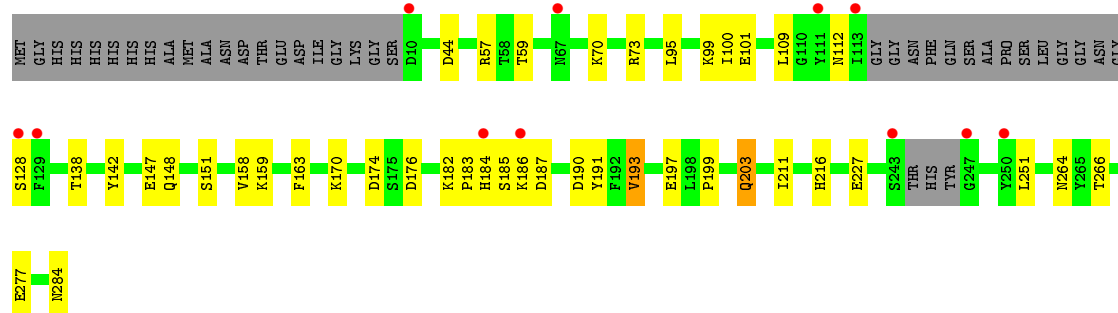


- Molecule 1: Gamma-hemolysin component C

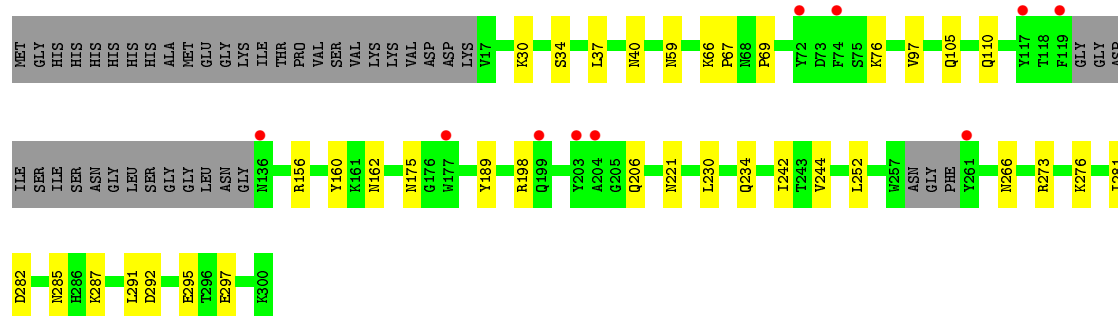
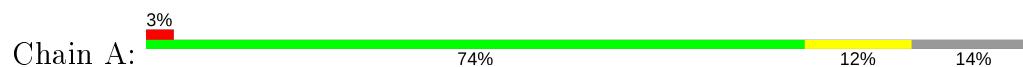


- Molecule 1: Gamma-hemolysin component C

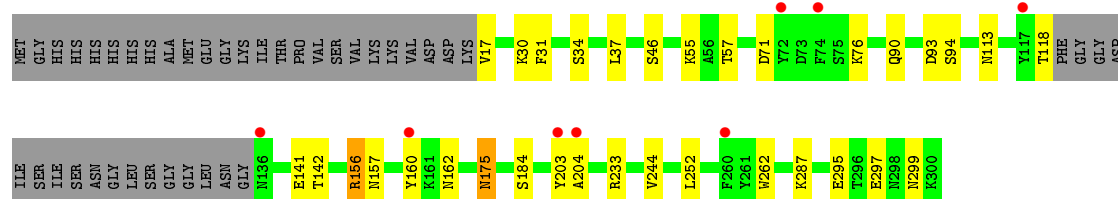
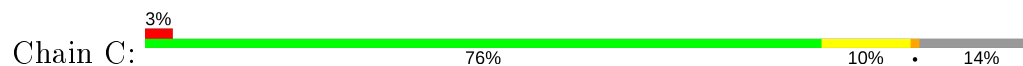




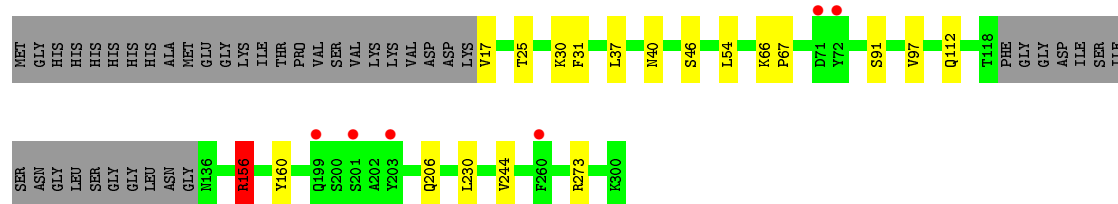
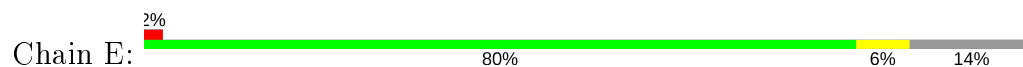
• Molecule 2: Gamma-hemolysin component B



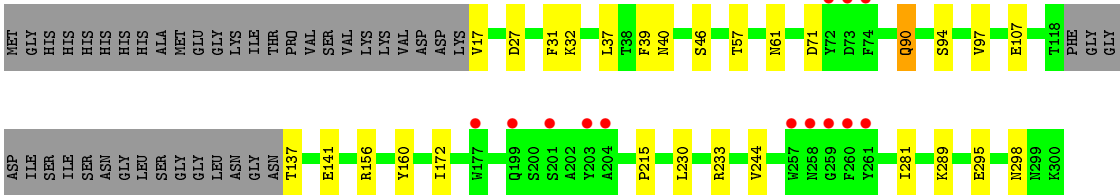
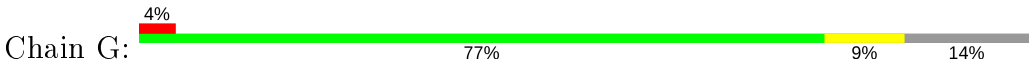
• Molecule 2: Gamma-hemolysin component B



• Molecule 2: Gamma-hemolysin component B



• Molecule 2: Gamma-hemolysin component B



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.31Å 193.16Å 116.38Å 90.00° 118.94° 90.00°	Depositor
Resolution (Å)	48.30 – 2.40 48.30 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.30-2.40) 99.6 (48.30-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.182 , 0.223 0.185 , 0.225	Depositor DCC
$R_{free}$ test set	2000 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	34827	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.69% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	B	0.66	0/2156	0.73	0/2910
1	D	0.68	0/2156	0.71	0/2910
1	F	0.68	0/2134	0.69	0/2878
1	H	0.69	0/2160	0.70	0/2915
2	A	0.66	0/2230	0.66	0/3014
2	C	0.66	0/2243	0.69	1/3033 (0.0%)
2	E	0.65	0/2243	0.69	2/3033 (0.1%)
2	G	0.66	0/2235	0.67	0/3022
All	All	0.67	0/17557	0.69	3/23715 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	156	ARG	NE-CZ-NH2	-6.82	116.89	120.30
2	E	156	ARG	NE-CZ-NH1	6.21	123.40	120.30
2	C	156	ARG	NE-CZ-NH1	5.16	122.88	120.30

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	B	2106	2050	2043	37	0
1	D	2106	2050	2043	26	0
1	F	2086	2033	2027	24	0
1	H	2110	2053	2046	31	0
2	A	2176	2083	2078	23	0
2	C	2188	2093	2088	26	0
2	E	2188	2093	2088	15	0
2	G	2180	2087	2082	23	0
3	A	8	14	14	0	0
3	C	8	14	14	0	0
3	E	8	14	14	0	0
3	G	8	14	14	0	0
4	A	120	0	0	11	0
4	B	140	0	0	13	0
4	C	122	0	0	12	0
4	D	141	0	0	5	0
4	E	118	0	0	5	1
4	F	151	0	0	5	0
4	G	117	0	0	12	1
4	H	148	0	0	9	1
All	All	18229	16598	16551	188	2

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 6.

All (188) 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:C:17:VAL:N	4:C:604:HOH:O	1.83	1.11
2:E:40:ASN:ND2	4:E:591:HOH:O	1.83	1.09
2:E:17:VAL:N	4:E:589:HOH:O	1.85	1.09
2:A:156:ARG:NH1	4:A:560:HOH:O	1.85	1.07
1:H:203:GLN:NE2	4:H:410:HOH:O	1.84	1.06
1:D:242:ARG:NH1	1:D:252:ASP:OD2	1.89	1.04
2:E:156:ARG:NH1	4:E:605:HOH:O	1.91	1.00
1:D:277:GLU:OE1	4:D:403:HOH:O	1.82	0.97
1:B:263:ARG:NH1	4:B:400:HOH:O	1.99	0.96
2:C:175:ASN:OD1	4:C:621:HOH:O	1.83	0.95
1:D:204:SER:O	2:E:156:ARG:NH2	2.00	0.94
2:E:206:GLN:OE1	4:E:588:HOH:O	1.84	0.93
2:A:30:LYS:NZ	4:A:603:HOH:O	2.06	0.89
1:H:190:ASP:OD2	4:H:447:HOH:O	1.92	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:141:GLU:OE2	4:G:608:HOH:O	1.93	0.87
1:F:10:ASP:N	4:F:408:HOH:O	2.08	0.85
2:G:40:ASN:ND2	4:G:611:HOH:O	2.10	0.85
2:G:17:VAL:N	4:G:573:HOH:O	2.09	0.84
1:B:263:ARG:NH1	4:B:428:HOH:O	2.10	0.84
1:D:101:GLU:OE1	4:D:325:HOH:O	1.97	0.82
1:H:148:GLN:OE1	4:H:359:HOH:O	1.98	0.82
2:E:17:VAL:N	4:E:608:HOH:O	2.13	0.79
1:F:183:PRO:O	1:F:185:SER:N	2.19	0.75
2:A:69:PRO:O	2:A:206:GLN:NE2	2.20	0.75
2:G:289:LYS:NZ	4:G:546:HOH:O	2.08	0.75
2:A:287:LYS:NZ	4:A:613:HOH:O	2.19	0.74
2:G:90:GLN:NE2	4:G:602:HOH:O	2.05	0.74
2:C:71:ASP:O	4:C:587:HOH:O	2.05	0.73
1:F:148:GLN:HG3	4:F:330:HOH:O	1.87	0.73
2:C:118:THR:O	4:C:610:HOH:O	2.07	0.72
1:D:147:GLU:OE2	1:D:159:LYS:NZ	2.23	0.72
2:C:90:GLN:HG3	4:C:515:HOH:O	1.88	0.71
2:A:292:ASP:OD2	4:A:501:HOH:O	2.08	0.71
2:A:156:ARG:NH2	4:A:612:HOH:O	2.24	0.71
2:A:175:ASN:ND2	4:A:620:HOH:O	2.24	0.70
2:A:105:GLN:OE1	4:A:572:HOH:O	2.09	0.70
1:D:264:ASN:O	1:D:284:ASN:ND2	2.25	0.70
1:H:277:GLU:OE1	4:H:409:HOH:O	2.10	0.70
2:G:17:VAL:N	4:G:511:HOH:O	2.24	0.69
1:H:284:ASN:O	4:H:301:HOH:O	2.11	0.69
2:C:34:SER:OG	4:C:518:HOH:O	2.10	0.69
1:H:101:GLU:OE1	4:H:331:HOH:O	2.12	0.67
1:B:70:LYS:NZ	4:B:393:HOH:O	2.26	0.66
2:C:287:LYS:NZ	4:C:616:HOH:O	2.29	0.65
2:A:34:SER:OG	4:A:519:HOH:O	2.12	0.64
1:B:148:GLN:OE1	4:B:435:HOH:O	2.15	0.64
1:B:101:GLU:OE1	4:B:399:HOH:O	2.15	0.64
1:F:44:ASP:OD1	4:F:339:HOH:O	2.15	0.63
1:B:184:HIS:N	4:B:346:HOH:O	2.04	0.62
1:B:263:ARG:NE	4:B:421:HOH:O	2.21	0.61
2:C:37:LEU:HD21	2:C:244:VAL:HG21	1.82	0.61
2:A:40:ASN:ND2	4:A:548:HOH:O	2.06	0.61
1:B:264:ASN:O	1:B:284:ASN:ND2	2.34	0.60
1:B:141:ASN:ND2	4:B:330:HOH:O	1.99	0.60
1:F:44:ASP:HB2	1:F:216:HIS:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:ALA:N	4:C:587:HOH:O	2.36	0.59
2:G:107:GLU:OE1	4:G:572:HOH:O	2.16	0.59
1:H:112:ASN:O	1:H:128:SER:N	2.36	0.58
1:H:264:ASN:O	1:H:284:ASN:ND2	2.36	0.58
1:F:63:TYR:HB3	1:F:69:VAL:HG23	1.85	0.58
1:F:193:VAL:HG13	1:F:197:GLU:HB2	1.85	0.57
1:F:57:ARG:H	2:G:156:ARG:HH12	1.51	0.57
2:A:110:GLN:HG2	1:H:138:THR:HG22	1.86	0.57
2:A:266:ASN:O	4:A:540:HOH:O	2.17	0.56
2:C:93:ASP:OD2	4:C:515:HOH:O	2.17	0.56
1:F:37:LYS:NZ	4:F:348:HOH:O	2.14	0.56
2:A:276:LYS:NZ	4:A:502:HOH:O	2.27	0.56
1:B:57:ARG:HA	2:C:156:ARG:HH22	1.70	0.55
1:F:20:LYS:HE2	1:F:280:VAL:HG21	1.88	0.55
1:H:193:VAL:HG13	1:H:197:GLU:HB2	1.88	0.55
1:H:44:ASP:HB2	1:H:216:HIS:HB3	1.89	0.55
2:G:137:THR:N	4:G:579:HOH:O	2.39	0.54
1:D:44:ASP:HB2	1:D:216:HIS:HB3	1.89	0.53
2:C:94:SER:HB2	2:C:233:ARG:HD3	1.90	0.53
2:E:25:THR:HG21	1:F:151:SER:CB	2.39	0.52
1:H:183:PRO:HB3	1:H:251:LEU:HD13	1.91	0.52
1:B:217:GLU:OE1	4:B:437:HOH:O	2.19	0.52
1:F:183:PRO:HB3	1:F:251:LEU:HD13	1.91	0.51
2:G:298:ASN:ND2	4:G:532:HOH:O	2.43	0.51
2:A:30:LYS:HE2	2:A:295:GLU:OE2	2.11	0.51
2:G:37:LEU:HD21	2:G:244:VAL:HG21	1.92	0.51
2:E:37:LEU:HD21	2:E:244:VAL:HG21	1.92	0.51
2:G:71:ASP:OD2	4:G:550:HOH:O	2.19	0.51
1:H:73:ARG:HD2	4:H:328:HOH:O	2.11	0.51
1:H:184:HIS:CD2	1:H:186:LYS:H	2.29	0.50
2:C:55:LYS:HG2	4:C:536:HOH:O	2.12	0.50
1:B:34:ASP:OD2	1:B:49:LYS:HE3	2.11	0.50
1:B:263:ARG:NH2	4:B:421:HOH:O	2.44	0.50
1:B:184:HIS:NE2	1:B:186:LYS:HA	2.26	0.49
1:D:242:ARG:O	1:D:250:TYR:N	2.40	0.49
1:F:57:ARG:N	2:G:156:ARG:HH12	2.10	0.49
2:C:113:ASN:ND2	2:C:141:GLU:OE1	2.43	0.49
1:F:83:LYS:NZ	4:F:448:HOH:O	2.07	0.49
1:B:44:ASP:HB2	1:B:216:HIS:HB3	1.93	0.49
2:E:25:THR:HG21	1:F:151:SER:HB3	1.95	0.48
2:A:282:ASP:OD2	2:A:285:ASN:ND2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASN:O	4:B:410:HOH:O	2.20	0.48
2:C:30:LYS:NZ	2:C:295:GLU:OE2	2.35	0.48
1:D:34:ASP:OD2	1:D:49:LYS:HE3	2.12	0.48
2:E:97:VAL:HG22	2:E:230:LEU:HD22	1.95	0.48
2:G:57:THR:HB	4:G:516:HOH:O	2.12	0.48
1:B:69:VAL:HG22	1:B:240:ILE:HG23	1.95	0.47
2:G:281:ILE:N	2:G:281:ILE:HD12	2.29	0.47
2:A:273:ARG:NH1	2:A:297:GLU:HB2	2.28	0.47
1:D:109:LEU:HD11	1:D:129:PHE:CZ	2.48	0.47
1:B:184:HIS:CD2	1:B:186:LYS:H	2.33	0.47
1:B:169:GLN:HG2	2:C:141:GLU:OE2	2.15	0.46
2:A:97:VAL:HG22	2:A:230:LEU:CD2	2.45	0.46
1:B:10:ASP:N	1:B:10:ASP:OD1	2.46	0.46
1:B:185:SER:O	1:B:186:LYS:HB2	2.14	0.46
1:F:69:VAL:HG12	1:F:240:ILE:HG23	1.97	0.46
1:B:20:LYS:HE2	1:B:280:VAL:HG21	1.96	0.46
1:F:95:LEU:HB2	1:F:211:ILE:HG22	1.96	0.46
2:G:94:SER:HB2	2:G:233:ARG:HD3	1.97	0.46
2:C:17:VAL:N	4:C:613:HOH:O	2.49	0.46
1:H:95:LEU:HB2	1:H:211:ILE:HG22	1.97	0.46
1:D:95:LEU:HB2	1:D:211:ILE:HG22	1.98	0.46
2:G:32:LYS:HB2	2:G:61:ASN:HB3	1.98	0.46
1:B:183:PRO:HA	1:B:184:HIS:HA	1.66	0.45
2:A:189:TYR:CZ	2:A:198:ARG:HD3	2.51	0.45
1:D:13:ILE:O	2:E:46:SER:HB2	2.16	0.45
1:B:70:LYS:HG2	1:B:188:PRO:HB3	1.99	0.45
2:A:37:LEU:HD21	2:A:244:VAL:HG21	1.99	0.45
2:G:97:VAL:HG22	2:G:230:LEU:CD2	2.47	0.45
1:B:260:PHE:HB3	1:B:263:ARG:HD3	1.98	0.45
1:B:83:LYS:HB3	1:B:153:SER:HB2	1.97	0.45
1:D:136:SER:HB3	2:E:112:GLN:HG3	1.97	0.44
1:H:147:GLU:OE2	1:H:159:LYS:CE	2.66	0.44
1:D:93:ASN:OD1	1:D:97:LYS:NZ	2.47	0.44
2:E:31:PHE:CE1	2:E:273:ARG:HD2	2.53	0.44
2:A:76:LYS:HD2	2:A:252:LEU:HD11	2.00	0.44
1:B:163:PHE:CE1	1:B:199:PRO:HG3	2.53	0.44
2:C:204:ALA:HB2	2:C:262:TRP:CH2	2.53	0.44
1:D:184:HIS:N	4:D:366:HOH:O	2.36	0.44
1:F:163:PHE:CE1	1:F:199:PRO:HG3	2.53	0.44
1:F:112:ASN:HB2	1:F:128:SER:HB3	1.99	0.44
1:B:266:THR:H	1:B:284:ASN:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:ARG:NH1	4:H:356:HOH:O	2.43	0.44
2:C:142:THR:HG23	1:D:108:THR:HG22	1.99	0.44
1:D:266:THR:H	1:D:284:ASN:HB2	1.83	0.44
1:D:73:ARG:HD2	4:D:317:HOH:O	2.17	0.44
1:H:183:PRO:HA	1:H:184:HIS:HA	1.79	0.43
1:H:57:ARG:O	1:H:59:THR:HG23	2.18	0.43
1:D:99:LYS:HE2	1:D:99:LYS:HA	2.01	0.43
1:D:184:HIS:CD2	1:D:186:LYS:H	2.36	0.43
1:H:147:GLU:OE2	1:H:159:LYS:HE2	2.18	0.43
1:B:166:GLU:OE2	1:D:133:LYS:NZ	2.50	0.43
2:G:172:ILE:HG23	2:G:215:PRO:HG3	2.00	0.43
4:G:547:HOH:O	1:H:100:ILE:HD13	2.19	0.43
1:B:13:ILE:O	2:C:46:SER:HB2	2.19	0.43
2:C:297:GLU:OE2	2:C:299:ASN:ND2	2.50	0.43
1:H:70:LYS:HD2	1:H:191:TYR:CE2	2.54	0.43
2:C:57:THR:HB	4:C:539:HOH:O	2.17	0.42
2:A:59:ASN:OD1	2:A:221:ASN:HB3	2.18	0.42
1:B:57:ARG:H	2:C:156:ARG:NH2	2.17	0.42
2:C:31:PHE:CE2	2:C:295:GLU:HB3	2.55	0.42
1:D:87:LYS:HB2	1:D:87:LYS:NZ	2.33	0.42
2:G:31:PHE:CE2	2:G:295:GLU:HB3	2.53	0.42
2:G:37:LEU:HB3	2:G:39:PHE:CE2	2.54	0.42
1:H:142:TYR:HB3	1:H:158:VAL:HG12	2.01	0.42
1:B:248:ASN:N	1:B:248:ASN:HD22	2.17	0.42
2:A:66:LYS:HB2	2:A:67:PRO:HD2	2.01	0.42
1:F:231:GLY:HA3	1:F:264:ASN:HA	2.00	0.42
2:A:242:ILE:HD12	2:A:281:ILE:HG13	2.01	0.42
1:H:95:LEU:HB2	1:H:211:ILE:CG2	2.50	0.42
2:C:76:LYS:HD3	2:C:252:LEU:HD11	2.02	0.42
2:G:27:ASP:OD2	1:H:151:SER:HB3	2.20	0.41
1:B:49:LYS:NZ	4:B:416:HOH:O	2.53	0.41
1:H:170:LYS:HG3	1:H:174:ASP:OD2	2.20	0.41
1:H:163:PHE:CE1	1:H:199:PRO:HG3	2.55	0.41
2:C:157:ASN:O	2:C:162:ASN:ND2	2.53	0.41
1:B:182:LYS:HB2	1:B:190:ASP:HB3	2.03	0.41
1:B:95:LEU:HB2	1:B:211:ILE:HG22	2.02	0.41
1:D:70:LYS:HB2	1:D:191:TYR:CD2	2.55	0.41
1:F:57:ARG:O	1:F:59:THR:HG23	2.21	0.41
1:F:13:ILE:O	2:G:46:SER:HB2	2.21	0.41
1:B:44:ASP:OD1	4:B:380:HOH:O	2.20	0.41
1:F:80:ILE:HG13	1:F:210:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:185:SER:C	1:H:187:ASP:H	2.24	0.41
1:D:30:ASN:OD1	1:D:52:GLY:HA2	2.21	0.40
1:H:266:THR:H	1:H:284:ASN:HB2	1.85	0.40
2:E:66:LYS:HB2	2:E:67:PRO:HD2	2.03	0.40
1:D:183:PRO:HA	1:D:184:HIS:HA	1.82	0.40
1:H:182:LYS:HB2	1:H:190:ASP:HB3	2.03	0.40
1:H:227:GLU:HG2	4:H:321:HOH:O	2.21	0.40
2:E:25:THR:HG21	1:F:151:SER:HB2	2.02	0.40
1:B:83:LYS:NZ	1:B:227:GLU:OE2	2.52	0.40
1:D:66:THR:O	4:D:399:HOH:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:505:HOH:O	4:H:312:HOH:O[4_545]	2.03	0.17
4:G:501:HOH:O	4:G:501:HOH:O[2_555]	2.06	0.14

## 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	B	251/296 (85%)	240 (96%)	10 (4%)	1 (0%)	34	48
1	D	251/296 (85%)	243 (97%)	8 (3%)	0	100	100
1	F	247/296 (83%)	238 (96%)	9 (4%)	0	100	100
1	H	252/296 (85%)	246 (98%)	6 (2%)	0	100	100
2	A	259/309 (84%)	250 (96%)	9 (4%)	0	100	100
2	C	263/309 (85%)	252 (96%)	11 (4%)	0	100	100
2	E	263/309 (85%)	254 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	262/309 (85%)	253 (97%)	9 (3%)	0	100	100
All	All	2048/2420 (85%)	1976 (96%)	71 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	LYS

### 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	B	237/264 (90%)	230 (97%)	7 (3%)	41	61
1	D	237/264 (90%)	234 (99%)	3 (1%)	69	84
1	F	234/264 (89%)	227 (97%)	7 (3%)	41	61
1	H	237/264 (90%)	232 (98%)	5 (2%)	53	72
2	A	237/271 (88%)	233 (98%)	4 (2%)	60	78
2	C	238/271 (88%)	234 (98%)	4 (2%)	60	78
2	E	238/271 (88%)	233 (98%)	5 (2%)	53	72
2	G	237/271 (88%)	235 (99%)	2 (1%)	81	91
All	All	1895/2140 (89%)	1858 (98%)	37 (2%)	55	74

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	90	SER
1	B	107	GLN
1	B	128	SER
1	B	129	PHE
1	B	185	SER
1	B	248	ASN
1	B	251	LEU

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Mol	Chain	Res	Type
2	A	160	TYR
2	A	162	ASN
2	A	234	GLN
2	A	291	LEU
2	C	160	TYR
2	C	175	ASN
2	C	184	SER
2	C	203	TYR
1	D	147	GLU
1	D	174	ASP
1	D	203	GLN
2	E	30	LYS
2	E	54	LEU
2	E	91	SER
2	E	156	ARG
2	E	160	TYR
1	F	22	SER
1	F	133	LYS
1	F	148	GLN
1	F	174	ASP
1	F	193	VAL
1	F	250	TYR
1	F	251	LEU
2	G	90	GLN
2	G	160	TYR
1	H	99	LYS
1	H	109	LEU
1	H	176	ASP
1	H	193	VAL
1	H	203	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	238	HIS
2	A	206	GLN
1	H	184	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are 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	$\# Z  > 2$
3	MPD	A	401	-	7,7,7	0.59	0	9,10,10	0.75	0
3	MPD	G	401	-	7,7,7	0.47	0	9,10,10	0.59	0
3	MPD	E	401	-	7,7,7	0.38	0	9,10,10	0.51	0
3	MPD	C	401	-	7,7,7	0.52	0	9,10,10	0.79	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
3	MPD	A	401	-	-	3/5/5/5	-
3	MPD	G	401	-	-	2/5/5/5	-
3	MPD	E	401	-	-	0/5/5/5	-
3	MPD	C	401	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	MPD	C2-C3-C4-O4
3	A	401	MPD	O2-C2-C3-C4
3	A	401	MPD	C1-C2-C3-C4
3	C	401	MPD	C1-C2-C3-C4
3	G	401	MPD	C2-C3-C4-C5
3	G	401	MPD	C2-C3-C4-O4

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	B	257/296 (86%)	0.04	8 (3%)	49	47	17, 32, 67, 80	0
1	D	257/296 (86%)	0.00	5 (1%)	66	64	17, 31, 63, 77	0
1	F	255/296 (86%)	0.02	8 (3%)	49	47	17, 32, 66, 77	0
1	H	258/296 (87%)	0.07	11 (4%)	35	33	16, 32, 68, 91	0
2	A	265/309 (85%)	0.10	10 (3%)	40	39	18, 35, 71, 85	0
2	C	267/309 (86%)	0.15	8 (2%)	50	49	19, 34, 65, 79	0
2	E	267/309 (86%)	0.06	6 (2%)	62	60	20, 34, 68, 79	0
2	G	266/309 (86%)	0.11	13 (4%)	29	28	20, 35, 67, 81	0
All	All	2092/2420 (86%)	0.07	69 (3%)	46	45	16, 33, 67, 91	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	247	GLY	6.7
2	E	260	PHE	5.4
2	G	260	PHE	4.9
2	G	72	TYR	3.9
2	A	119	PHE	3.9
1	B	184	HIS	3.9
1	B	111	TYR	3.8
2	C	136	ASN	3.8
1	H	243	SER	3.7
2	A	117	TYR	3.6
1	D	184	HIS	3.6
2	A	72	TYR	3.6
1	H	184	HIS	3.6
2	A	136	ASN	3.6
1	F	10	ASP	3.5
1	F	127	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	A	203	TYR	3.3
2	A	261	TYR	3.2
2	G	259	GLY	3.2
1	F	66	THR	3.1
2	C	204	ALA	3.1
1	H	111	TYR	3.1
2	G	203	TYR	3.1
1	H	250	TYR	3.1
2	C	72	TYR	3.0
2	E	72	TYR	3.0
1	H	128	SER	2.9
2	C	260	PHE	2.8
2	C	203	TYR	2.8
2	G	74	PHE	2.7
2	C	117	TYR	2.7
2	G	199	GLN	2.7
2	E	199	GLN	2.7
2	A	74	PHE	2.6
1	F	129	PHE	2.6
1	B	65	LYS	2.5
2	C	74	PHE	2.5
1	B	10	ASP	2.5
1	H	67	ASN	2.5
1	B	129	PHE	2.5
1	F	250	TYR	2.5
2	G	204	ALA	2.5
2	A	199	GLN	2.4
1	F	111	TYR	2.4
1	D	65	LYS	2.4
2	G	73	ASP	2.4
2	A	204	ALA	2.4
2	E	203	TYR	2.4
1	D	66	THR	2.3
2	E	71	ASP	2.3
1	H	10	ASP	2.3
1	B	113	ILE	2.3
1	F	65	LYS	2.3
1	D	129	PHE	2.3
1	H	129	PHE	2.3
1	F	68	HIS	2.2
1	H	186	LYS	2.2
2	G	261	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	201	SER	2.2
2	G	258	ASN	2.2
2	G	177	TRP	2.2
2	G	257	TRP	2.1
2	A	177	TRP	2.1
1	D	113	ILE	2.1
1	H	113	ILE	2.1
2	G	201	SER	2.1
2	C	160	TYR	2.1
1	B	22	SER	2.1
1	B	186	LYS	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 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
3	MPD	A	401	8/8	0.76	0.36	68,85,94,103	0
3	MPD	E	401	8/8	0.84	0.27	60,77,92,94	0
3	MPD	C	401	8/8	0.85	0.41	61,81,90,97	0
3	MPD	G	401	8/8	0.91	0.30	61,76,90,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.