



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:00 AM UTC

PDB ID : 4H56 / pdb_00004h56
Title : Crystal structure of the Clostridium perfringens NetB toxin in the membrane inserted form
Authors : Savva, C.G.; Fernandes da Costa, S.P.; Bokori-Brown, M.; Naylor, C.; Cole, A.R.; Moss, D.S.; Titball, R.W.; Basak, A.K.
Deposited on : 2012-09-18
Resolution : 3.90 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:

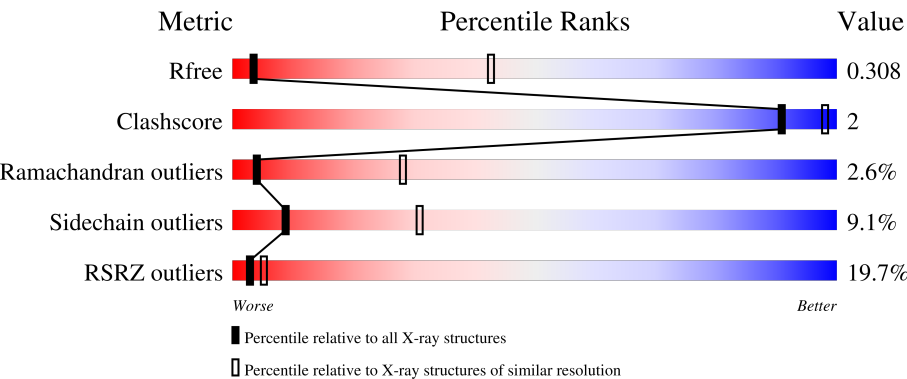
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	296	
1	B	296	
1	C	296	
1	D	296	
1	E	296	

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Mol	Chain	Length	Quality of chain
1	F	296	
1	G	296	
1	H	296	
1	I	296	
1	J	296	
1	K	296	
1	L	296	
1	M	296	
1	N	296	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27963 atoms, of which 0 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 Necrotic enteritis toxin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			1984	1239	335	406	4			
1	B	267	Total	C	N	O	S	0	0	0
			1977	1236	328	409	4			
1	C	267	Total	C	N	O	S	0	0	0
			1996	1247	337	409	3			
1	D	267	Total	C	N	O	S	0	0	0
			1988	1249	331	405	3			
1	E	267	Total	C	N	O	S	0	0	0
			1966	1232	331	399	4			
1	F	267	Total	C	N	O	S	0	0	0
			1983	1238	330	412	3			
1	G	267	Total	C	N	O	S	0	0	0
			1995	1252	331	408	4			
1	H	267	Total	C	N	O	S	0	0	0
			1996	1249	335	408	4			
1	I	267	Total	C	N	O	S	0	0	0
			2008	1259	336	410	3			
1	J	267	Total	C	N	O	S	0	0	0
			2009	1262	336	407	4			
1	K	267	Total	C	N	O	S	0	0	0
			2013	1267	334	408	4			
1	L	267	Total	C	N	O	S	0	0	0
			2023	1270	336	413	4			
1	M	267	Total	C	N	O	S	0	0	0
			2005	1259	332	410	4			
1	N	267	Total	C	N	O	S	0	0	0
			2020	1265	337	414	4			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A8ULG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP A8ULG6
A	-1	MET	-	expression tag	UNP A8ULG6
A	0	GLY	-	expression tag	UNP A8ULG6
B	-3	GLY	-	expression tag	UNP A8ULG6
B	-2	ALA	-	expression tag	UNP A8ULG6
B	-1	MET	-	expression tag	UNP A8ULG6
B	0	GLY	-	expression tag	UNP A8ULG6
C	-3	GLY	-	expression tag	UNP A8ULG6
C	-2	ALA	-	expression tag	UNP A8ULG6
C	-1	MET	-	expression tag	UNP A8ULG6
C	0	GLY	-	expression tag	UNP A8ULG6
D	-3	GLY	-	expression tag	UNP A8ULG6
D	-2	ALA	-	expression tag	UNP A8ULG6
D	-1	MET	-	expression tag	UNP A8ULG6
D	0	GLY	-	expression tag	UNP A8ULG6
E	-3	GLY	-	expression tag	UNP A8ULG6
E	-2	ALA	-	expression tag	UNP A8ULG6
E	-1	MET	-	expression tag	UNP A8ULG6
E	0	GLY	-	expression tag	UNP A8ULG6
F	-3	GLY	-	expression tag	UNP A8ULG6
F	-2	ALA	-	expression tag	UNP A8ULG6
F	-1	MET	-	expression tag	UNP A8ULG6
F	0	GLY	-	expression tag	UNP A8ULG6
G	-3	GLY	-	expression tag	UNP A8ULG6
G	-2	ALA	-	expression tag	UNP A8ULG6
G	-1	MET	-	expression tag	UNP A8ULG6
G	0	GLY	-	expression tag	UNP A8ULG6
H	-3	GLY	-	expression tag	UNP A8ULG6
H	-2	ALA	-	expression tag	UNP A8ULG6
H	-1	MET	-	expression tag	UNP A8ULG6
H	0	GLY	-	expression tag	UNP A8ULG6
I	-3	GLY	-	expression tag	UNP A8ULG6
I	-2	ALA	-	expression tag	UNP A8ULG6
I	-1	MET	-	expression tag	UNP A8ULG6
I	0	GLY	-	expression tag	UNP A8ULG6
J	-3	GLY	-	expression tag	UNP A8ULG6
J	-2	ALA	-	expression tag	UNP A8ULG6
J	-1	MET	-	expression tag	UNP A8ULG6
J	0	GLY	-	expression tag	UNP A8ULG6
K	-3	GLY	-	expression tag	UNP A8ULG6
K	-2	ALA	-	expression tag	UNP A8ULG6
K	-1	MET	-	expression tag	UNP A8ULG6

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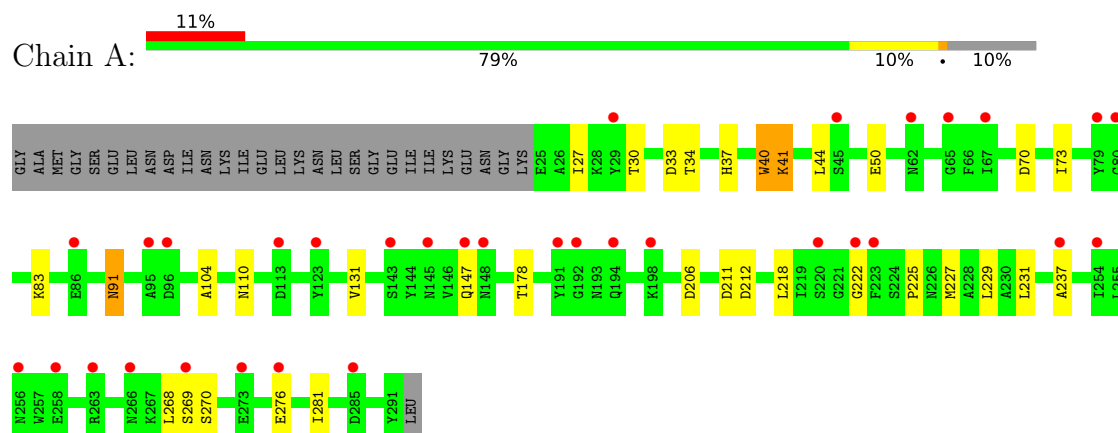
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Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP A8ULG6
L	-3	GLY	-	expression tag	UNP A8ULG6
L	-2	ALA	-	expression tag	UNP A8ULG6
L	-1	MET	-	expression tag	UNP A8ULG6
L	0	GLY	-	expression tag	UNP A8ULG6
M	-3	GLY	-	expression tag	UNP A8ULG6
M	-2	ALA	-	expression tag	UNP A8ULG6
M	-1	MET	-	expression tag	UNP A8ULG6
M	0	GLY	-	expression tag	UNP A8ULG6
N	-3	GLY	-	expression tag	UNP A8ULG6
N	-2	ALA	-	expression tag	UNP A8ULG6
N	-1	MET	-	expression tag	UNP A8ULG6
N	0	GLY	-	expression tag	UNP A8ULG6

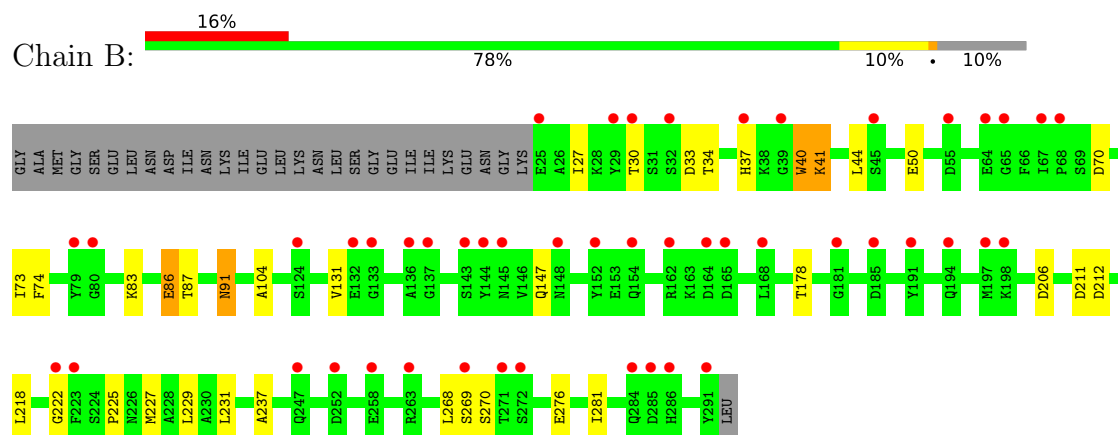
3 Residue-property plots [i](#)

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.

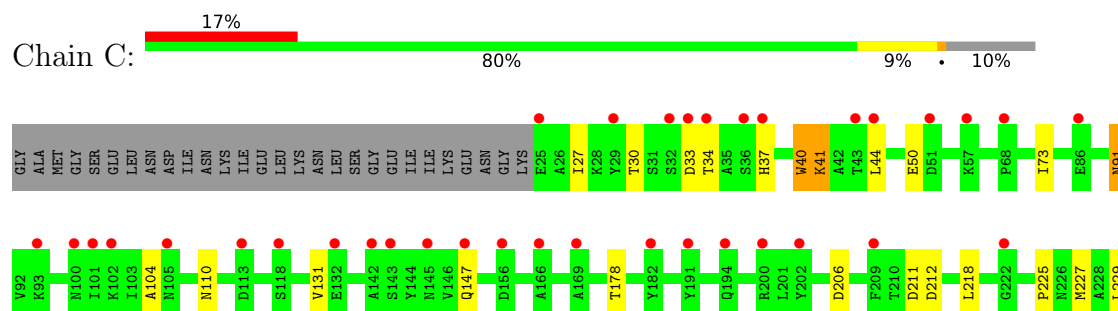
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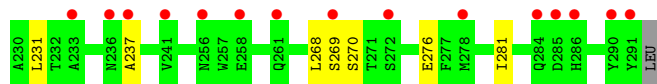


• Molecule 1: Necrotic enteritis toxin B

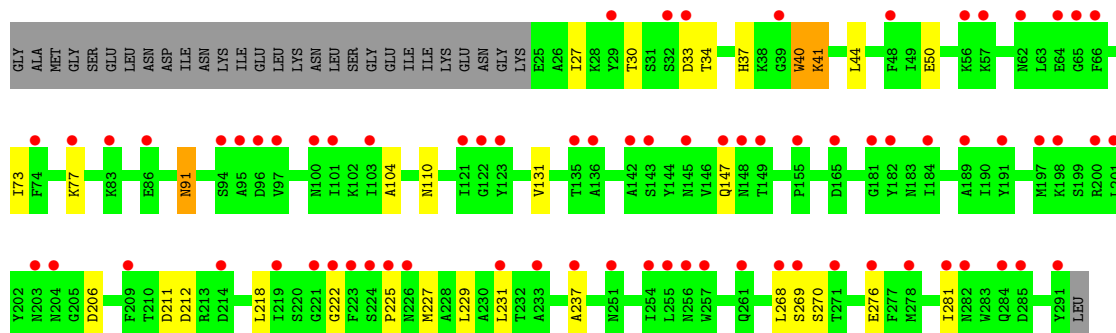
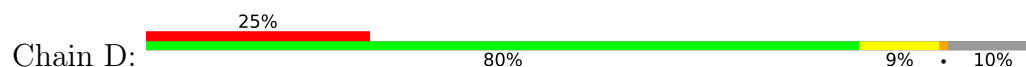


• Molecule 1: Necrotic enteritis toxin B

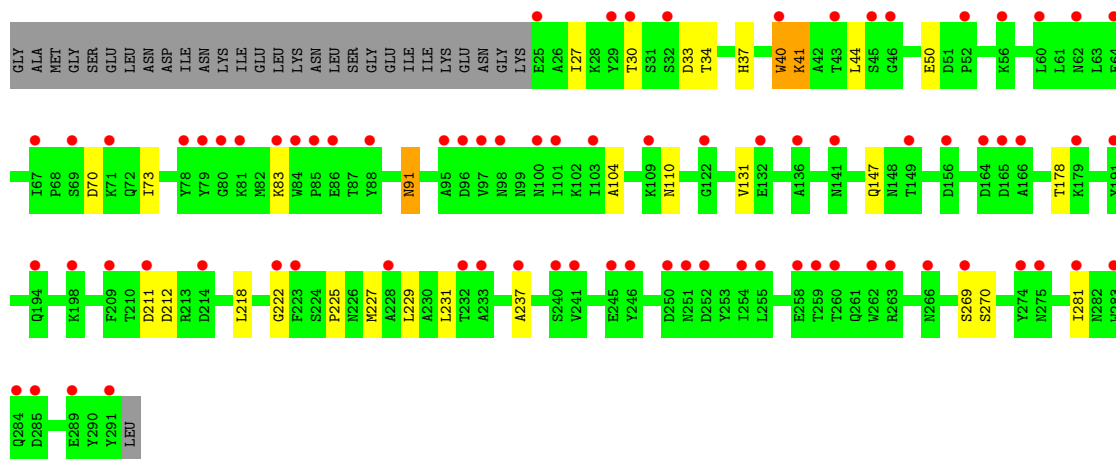
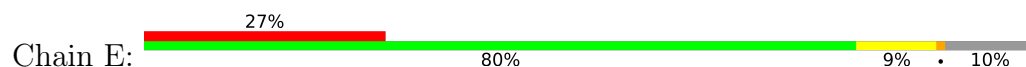




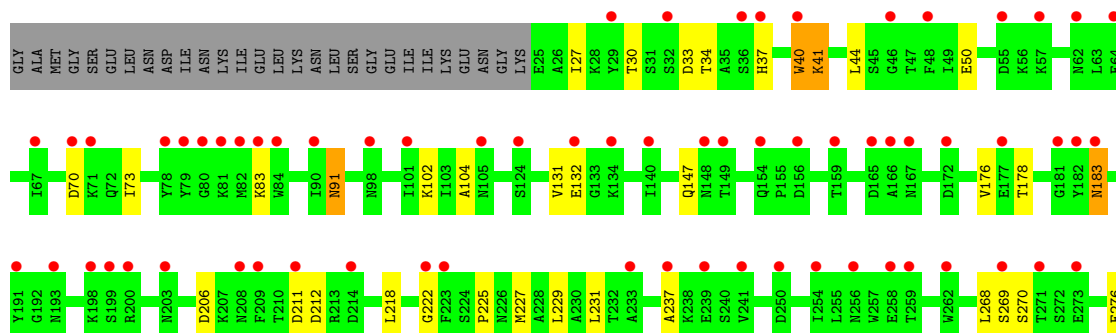
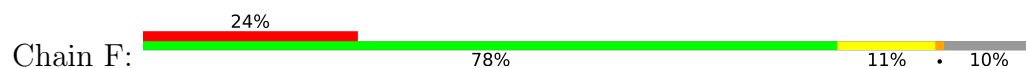
● Molecule 1: Necrotic enteritis toxin B

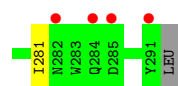


● Molecule 1: Necrotic enteritis toxin B

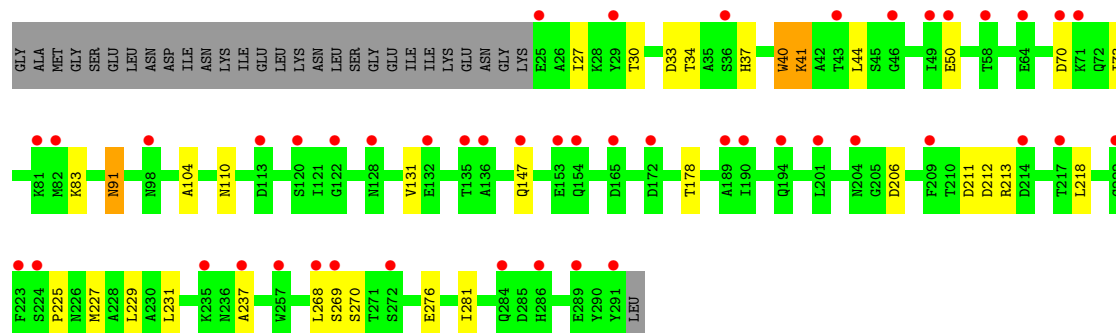
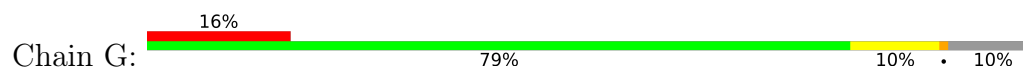


● Molecule 1: Necrotic enteritis toxin B

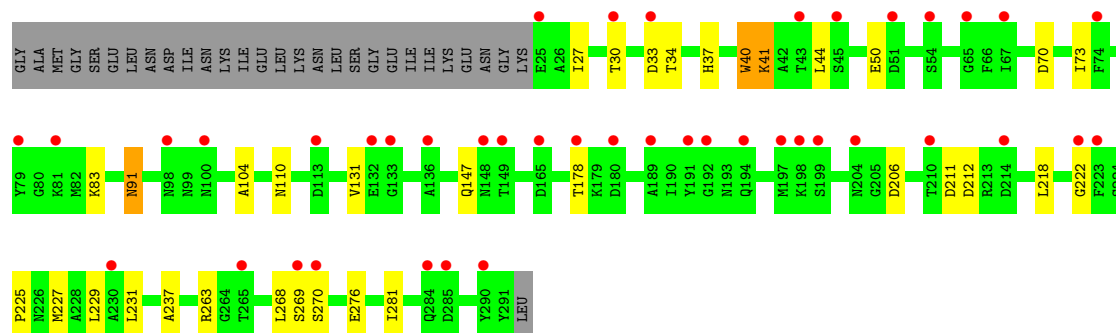
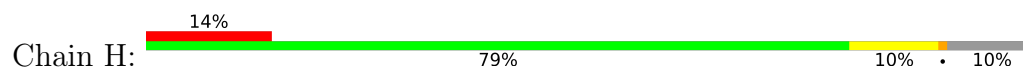




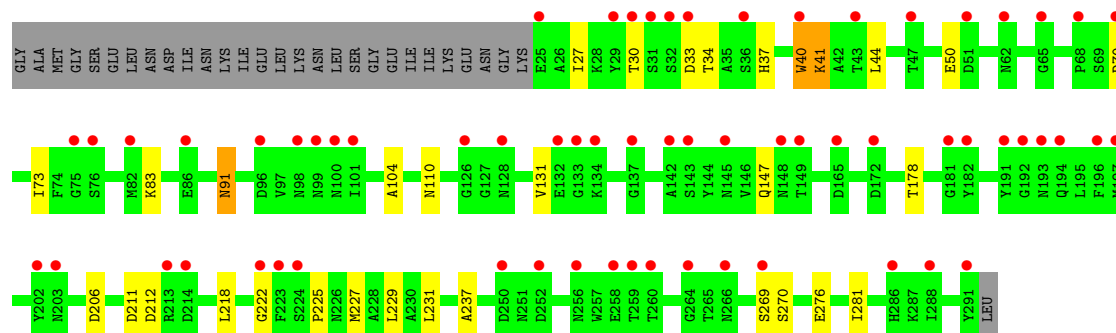
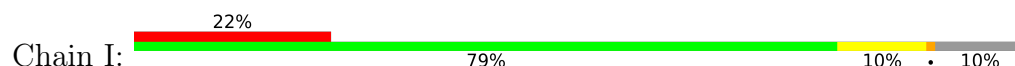
● Molecule 1: Necrotic enteritis toxin B



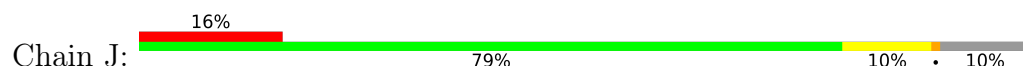
● Molecule 1: Necrotic enteritis toxin B

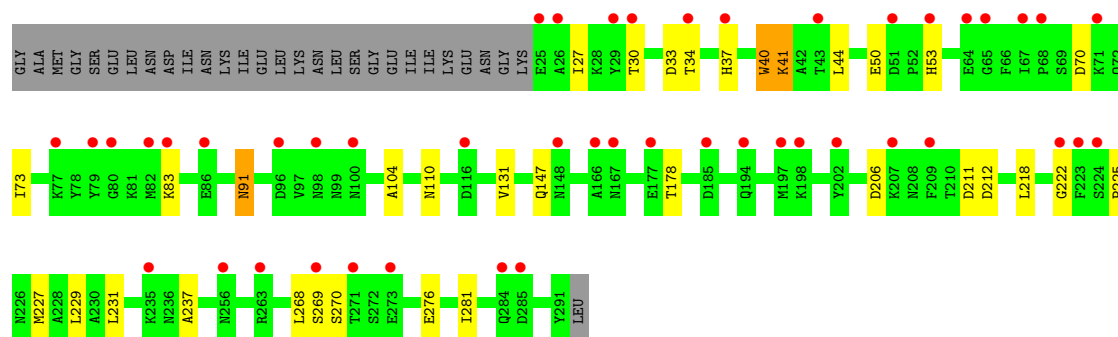


● Molecule 1: Necrotic enteritis toxin B

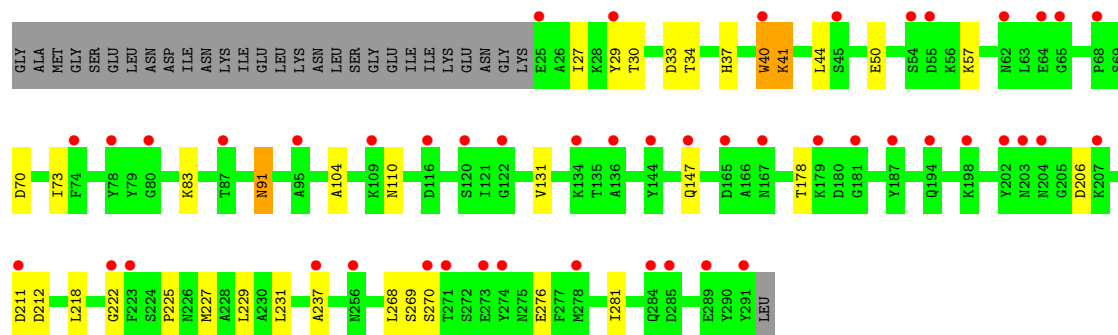
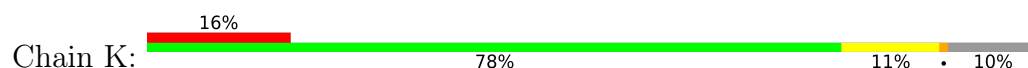


● Molecule 1: Necrotic enteritis toxin B

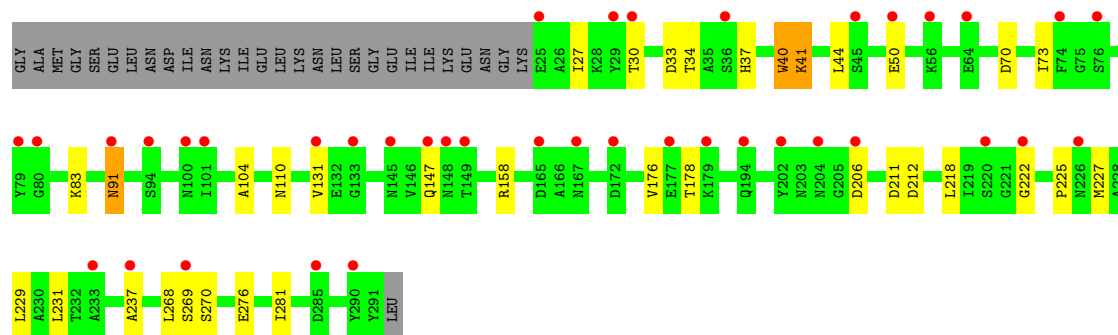
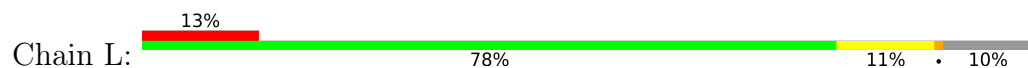




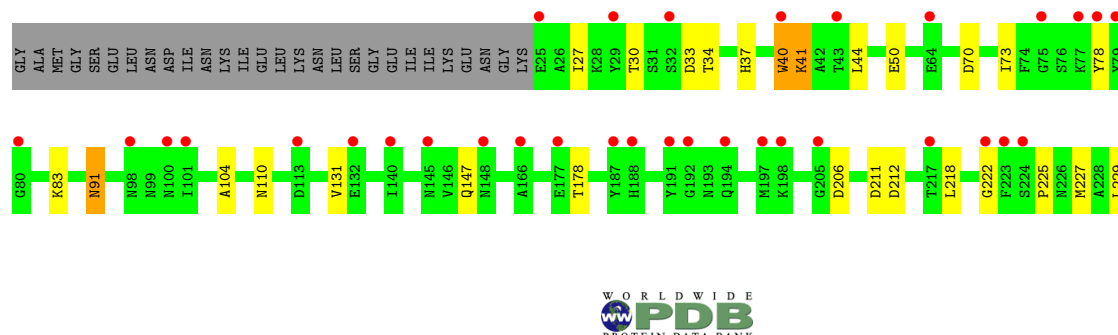
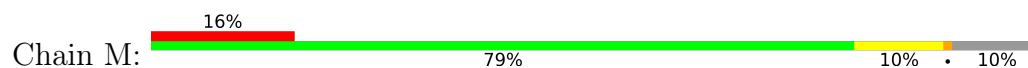
• Molecule 1: Necrotic enteritis toxin B

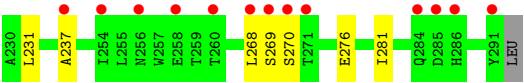


• Molecule 1: Necrotic enteritis toxin B

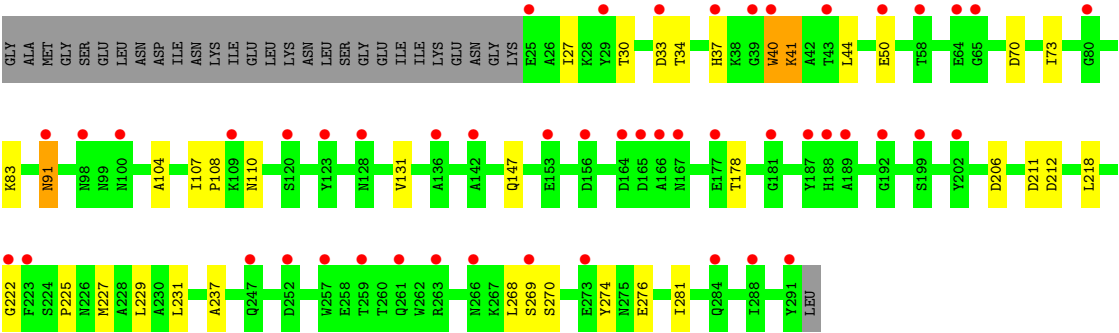
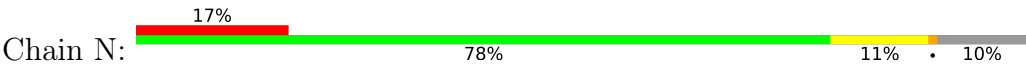


• Molecule 1: Necrotic enteritis toxin B





● Molecule 1: Necrotic enteritis toxin B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	313.23Å 168.04Å 160.46Å 90.00° 109.42° 90.00°	Depositor
Resolution (Å)	27.70 – 3.90 27.70 – 3.90	Depositor EDS
% Data completeness (in resolution range)	89.6 (27.70-3.90) 97.2 (27.70-3.90)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 3.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.284 , 0.309 0.284 , 0.308	Depositor DCC
R_{free} test set	3514 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	1.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	27963	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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	0.30	0/2025	0.63	0/2763
1	B	0.31	0/2019	0.63	0/2761
1	C	0.30	0/2039	0.62	0/2785
1	D	0.30	0/2033	0.63	0/2779
1	E	0.30	0/2009	0.63	0/2747
1	F	0.31	0/2025	0.63	0/2767
1	G	0.31	0/2040	0.63	0/2788
1	H	0.31	0/2040	0.63	0/2786
1	I	0.31	0/2053	0.63	0/2802
1	J	0.31	0/2053	0.63	0/2798
1	K	0.31	0/2058	0.63	0/2805
1	L	0.31	0/2068	0.64	0/2820
1	M	0.31	0/2051	0.63	0/2803
1	N	0.30	0/2064	0.63	0/2815
All	All	0.31	0/28577	0.63	0/39019

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 [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	1984	0	1765	7	0
1	B	1977	0	1728	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1996	0	1765	5	0
1	D	1988	0	1748	6	0
1	E	1966	0	1721	7	0
1	F	1983	0	1737	9	0
1	G	1995	0	1754	7	0
1	H	1996	0	1760	8	0
1	I	2008	0	1781	7	0
1	J	2009	0	1804	9	0
1	K	2013	0	1809	9	0
1	L	2023	0	1815	9	0
1	M	2005	0	1765	7	0
1	N	2020	0	1809	9	0
All	All	27963	0	24761	91	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 2.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:ASN:OD1	1:G:213:ARG:NE	2.24	0.70
1:F:176:VAL:O	1:F:183:ASN:ND2	2.27	0.68
1:C:110:ASN:ND2	1:D:222:GLY:O	2.35	0.60
1:B:74:PHE:HB3	1:N:274:TYR:CG	2.39	0.57
1:M:110:ASN:ND2	1:N:222:GLY:O	2.40	0.54
1:H:222:GLY:O	1:N:110:ASN:ND2	2.40	0.54
1:A:222:GLY:O	1:G:110:ASN:ND2	2.42	0.53
1:F:91:ASN:OD1	1:F:91:ASN:N	2.43	0.52
1:M:91:ASN:N	1:M:91:ASN:OD1	2.43	0.52
1:A:91:ASN:N	1:A:91:ASN:OD1	2.43	0.52
1:C:91:ASN:N	1:C:91:ASN:OD1	2.43	0.52
1:B:91:ASN:OD1	1:B:91:ASN:N	2.43	0.52
1:L:91:ASN:N	1:L:91:ASN:OD1	2.43	0.52
1:E:91:ASN:N	1:E:91:ASN:OD1	2.43	0.51
1:N:91:ASN:N	1:N:91:ASN:OD1	2.43	0.51
1:D:91:ASN:N	1:D:91:ASN:OD1	2.43	0.51
1:H:91:ASN:N	1:H:91:ASN:OD1	2.43	0.51
1:K:91:ASN:N	1:K:91:ASN:OD1	2.43	0.51
1:G:91:ASN:N	1:G:91:ASN:OD1	2.43	0.51
1:J:91:ASN:OD1	1:J:91:ASN:N	2.43	0.51
1:E:110:ASN:ND2	1:F:222:GLY:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASN:ND2	1:E:222:GLY:O	2.44	0.49
1:L:158:ARG:HG2	1:L:176:VAL:HG21	1.95	0.49
1:N:107:ILE:HG23	1:N:108:PRO:HA	1.95	0.48
1:I:91:ASN:N	1:I:91:ASN:OD1	2.46	0.48
1:A:110:ASN:ND2	1:B:222:GLY:O	2.48	0.46
1:J:110:ASN:ND2	1:K:222:GLY:O	2.48	0.46
1:I:110:ASN:ND2	1:J:222:GLY:O	2.49	0.46
1:N:211:ASP:OD1	1:N:212:ASP:N	2.50	0.45
1:C:211:ASP:OD1	1:C:212:ASP:N	2.51	0.44
1:D:211:ASP:OD1	1:D:212:ASP:N	2.51	0.44
1:H:263:ARG:O	1:H:263:ARG:HG3	2.16	0.44
1:L:158:ARG:HG2	1:L:176:VAL:CG2	2.47	0.44
1:M:211:ASP:OD1	1:M:212:ASP:N	2.51	0.44
1:G:211:ASP:OD1	1:G:212:ASP:N	2.51	0.44
1:F:211:ASP:OD1	1:F:212:ASP:N	2.50	0.44
1:E:70:ASP:OD1	1:E:83:LYS:NZ	2.51	0.44
1:N:70:ASP:OD1	1:N:83:LYS:NZ	2.51	0.44
1:F:40:TRP:O	1:F:41:LYS:CB	2.66	0.44
1:A:211:ASP:OD1	1:A:212:ASP:N	2.51	0.44
1:B:211:ASP:OD1	1:B:212:ASP:N	2.51	0.44
1:J:70:ASP:OD1	1:J:83:LYS:NZ	2.51	0.44
1:F:70:ASP:OD1	1:F:83:LYS:NZ	2.51	0.44
1:G:70:ASP:OD1	1:G:83:LYS:NZ	2.51	0.44
1:H:70:ASP:OD1	1:H:83:LYS:NZ	2.51	0.44
1:L:70:ASP:OD1	1:L:83:LYS:NZ	2.51	0.44
1:A:33:ASP:OD1	1:A:34:THR:N	2.51	0.43
1:H:211:ASP:OD1	1:H:212:ASP:N	2.51	0.43
1:I:70:ASP:OD1	1:I:83:LYS:NZ	2.51	0.43
1:J:211:ASP:OD1	1:J:212:ASP:N	2.51	0.43
1:E:211:ASP:OD1	1:E:212:ASP:N	2.51	0.43
1:K:70:ASP:OD1	1:K:83:LYS:NZ	2.51	0.43
1:L:211:ASP:OD1	1:L:212:ASP:N	2.51	0.43
1:C:33:ASP:OD1	1:C:34:THR:N	2.52	0.43
1:K:211:ASP:OD1	1:K:212:ASP:N	2.50	0.43
1:E:40:TRP:O	1:E:41:LYS:CB	2.66	0.43
1:F:176:VAL:O	1:F:183:ASN:CG	2.62	0.43
1:B:70:ASP:OD1	1:B:83:LYS:NZ	2.51	0.43
1:F:33:ASP:OD1	1:F:34:THR:N	2.51	0.43
1:G:33:ASP:OD1	1:G:34:THR:N	2.52	0.43
1:M:70:ASP:OD1	1:M:83:LYS:NZ	2.51	0.43
1:B:33:ASP:OD1	1:B:34:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:TRP:O	1:G:41:LYS:CB	2.66	0.43
1:H:40:TRP:O	1:H:41:LYS:CB	2.66	0.43
1:I:33:ASP:OD1	1:I:34:THR:N	2.52	0.43
1:I:211:ASP:OD1	1:I:212:ASP:N	2.51	0.43
1:M:33:ASP:OD1	1:M:34:THR:N	2.52	0.43
1:A:70:ASP:OD1	1:A:83:LYS:NZ	2.51	0.43
1:K:110:ASN:ND2	1:L:222:GLY:O	2.52	0.43
1:L:33:ASP:OD1	1:L:34:THR:N	2.52	0.43
1:J:33:ASP:OD1	1:J:34:THR:N	2.52	0.42
1:K:33:ASP:OD1	1:K:34:THR:N	2.52	0.42
1:N:33:ASP:OD1	1:N:34:THR:N	2.52	0.42
1:B:86:GLU:HG3	1:B:87:THR:HG22	2.01	0.42
1:C:40:TRP:O	1:C:41:LYS:CB	2.66	0.42
1:D:33:ASP:OD1	1:D:34:THR:N	2.51	0.42
1:E:33:ASP:OD1	1:E:34:THR:N	2.52	0.42
1:H:33:ASP:OD1	1:H:34:THR:N	2.52	0.42
1:H:110:ASN:ND2	1:I:222:GLY:O	2.52	0.42
1:J:53:HIS:CD2	1:K:29:TYR:CE2	3.08	0.42
1:J:53:HIS:HB3	1:K:29:TYR:HA	2.01	0.42
1:L:110:ASN:ND2	1:M:222:GLY:O	2.53	0.42
1:L:40:TRP:O	1:L:41:LYS:CB	2.68	0.41
1:N:40:TRP:O	1:N:41:LYS:CB	2.68	0.41
1:A:40:TRP:O	1:A:41:LYS:CB	2.69	0.41
1:D:40:TRP:O	1:D:41:LYS:CB	2.68	0.41
1:J:40:TRP:O	1:J:41:LYS:CB	2.68	0.41
1:K:40:TRP:O	1:K:41:LYS:CB	2.68	0.41
1:B:40:TRP:O	1:B:41:LYS:CB	2.69	0.41
1:M:40:TRP:O	1:M:41:LYS:CB	2.69	0.40
1:I:40:TRP:O	1:I:41:LYS:CB	2.68	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	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	4	28
1	B	265/296 (90%)	236 (89%)	22 (8%)	7 (3%)	4	28
1	C	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	4	28
1	D	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	4	28
1	E	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	4	28
1	F	265/296 (90%)	236 (89%)	22 (8%)	7 (3%)	4	28
1	G	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	4	28
1	H	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	4	28
1	I	265/296 (90%)	237 (89%)	21 (8%)	7 (3%)	4	28
1	J	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	4	28
1	K	265/296 (90%)	236 (89%)	22 (8%)	7 (3%)	4	28
1	L	265/296 (90%)	236 (89%)	22 (8%)	7 (3%)	4	28
1	M	265/296 (90%)	235 (89%)	23 (9%)	7 (3%)	4	28
1	N	265/296 (90%)	236 (89%)	22 (8%)	7 (3%)	4	28
All	All	3710/4144 (90%)	3297 (89%)	315 (8%)	98 (3%)	4	28

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	269	SER
1	B	41	LYS
1	B	269	SER
1	C	41	LYS
1	C	269	SER
1	D	41	LYS
1	D	269	SER
1	E	41	LYS
1	E	269	SER
1	F	37	HIS
1	F	41	LYS
1	F	269	SER
1	G	41	LYS
1	G	269	SER
1	H	41	LYS
1	H	269	SER
1	I	37	HIS
1	I	41	LYS

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Mol	Chain	Res	Type
1	I	269	SER
1	J	41	LYS
1	J	269	SER
1	K	41	LYS
1	K	269	SER
1	L	41	LYS
1	L	269	SER
1	M	41	LYS
1	M	269	SER
1	N	41	LYS
1	N	269	SER
1	A	37	HIS
1	A	237	ALA
1	B	37	HIS
1	B	237	ALA
1	C	37	HIS
1	C	237	ALA
1	D	37	HIS
1	D	237	ALA
1	E	37	HIS
1	E	237	ALA
1	F	237	ALA
1	G	37	HIS
1	G	237	ALA
1	H	37	HIS
1	H	237	ALA
1	I	237	ALA
1	J	37	HIS
1	J	237	ALA
1	K	37	HIS
1	K	237	ALA
1	L	37	HIS
1	L	237	ALA
1	M	37	HIS
1	M	237	ALA
1	N	37	HIS
1	N	237	ALA
1	A	40	TRP
1	A	104	ALA
1	B	40	TRP
1	B	104	ALA
1	C	40	TRP

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Mol	Chain	Res	Type
1	C	104	ALA
1	D	40	TRP
1	D	104	ALA
1	E	40	TRP
1	E	104	ALA
1	F	40	TRP
1	F	104	ALA
1	G	40	TRP
1	G	104	ALA
1	H	40	TRP
1	H	104	ALA
1	I	40	TRP
1	I	104	ALA
1	J	40	TRP
1	J	104	ALA
1	K	40	TRP
1	K	104	ALA
1	L	40	TRP
1	L	104	ALA
1	M	40	TRP
1	M	104	ALA
1	N	40	TRP
1	N	104	ALA
1	A	225	PRO
1	B	225	PRO
1	C	225	PRO
1	D	225	PRO
1	E	225	PRO
1	F	225	PRO
1	G	225	PRO
1	H	225	PRO
1	I	225	PRO
1	J	225	PRO
1	K	225	PRO
1	L	225	PRO
1	M	225	PRO
1	N	225	PRO

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	197/258 (76%)	179 (91%)	18 (9%)	9	31
1	B	194/258 (75%)	175 (90%)	19 (10%)	7	28
1	C	198/258 (77%)	180 (91%)	18 (9%)	9	31
1	D	195/258 (76%)	177 (91%)	18 (9%)	8	30
1	E	190/258 (74%)	175 (92%)	15 (8%)	11	36
1	F	196/258 (76%)	175 (89%)	21 (11%)	6	24
1	G	197/258 (76%)	179 (91%)	18 (9%)	9	31
1	H	197/258 (76%)	179 (91%)	18 (9%)	9	31
1	I	200/258 (78%)	183 (92%)	17 (8%)	10	33
1	J	201/258 (78%)	183 (91%)	18 (9%)	9	31
1	K	202/258 (78%)	183 (91%)	19 (9%)	8	29
1	L	205/258 (80%)	187 (91%)	18 (9%)	9	32
1	M	199/258 (77%)	180 (90%)	19 (10%)	8	29
1	N	205/258 (80%)	187 (91%)	18 (9%)	9	32
All	All	2776/3612 (77%)	2522 (91%)	254 (9%)	9	31

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	30	THR
1	A	44	LEU
1	A	50	GLU
1	A	73	ILE
1	A	91	ASN
1	A	131	VAL
1	A	147	GLN
1	A	178	THR
1	A	206	ASP
1	A	218	LEU
1	A	227	MET
1	A	229	LEU
1	A	231	LEU
1	A	268	LEU

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Mol	Chain	Res	Type
1	A	270	SER
1	A	276	GLU
1	A	281	ILE
1	B	27	ILE
1	B	30	THR
1	B	44	LEU
1	B	50	GLU
1	B	73	ILE
1	B	86	GLU
1	B	91	ASN
1	B	131	VAL
1	B	147	GLN
1	B	178	THR
1	B	206	ASP
1	B	218	LEU
1	B	227	MET
1	B	229	LEU
1	B	231	LEU
1	B	268	LEU
1	B	270	SER
1	B	276	GLU
1	B	281	ILE
1	C	27	ILE
1	C	30	THR
1	C	44	LEU
1	C	50	GLU
1	C	73	ILE
1	C	91	ASN
1	C	131	VAL
1	C	147	GLN
1	C	178	THR
1	C	206	ASP
1	C	218	LEU
1	C	227	MET
1	C	229	LEU
1	C	231	LEU
1	C	268	LEU
1	C	270	SER
1	C	276	GLU
1	C	281	ILE
1	D	27	ILE
1	D	30	THR

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Mol	Chain	Res	Type
1	D	44	LEU
1	D	50	GLU
1	D	73	ILE
1	D	77	LYS
1	D	91	ASN
1	D	131	VAL
1	D	147	GLN
1	D	206	ASP
1	D	218	LEU
1	D	227	MET
1	D	229	LEU
1	D	231	LEU
1	D	268	LEU
1	D	270	SER
1	D	276	GLU
1	D	281	ILE
1	E	27	ILE
1	E	30	THR
1	E	44	LEU
1	E	50	GLU
1	E	73	ILE
1	E	91	ASN
1	E	131	VAL
1	E	147	GLN
1	E	178	THR
1	E	218	LEU
1	E	227	MET
1	E	229	LEU
1	E	231	LEU
1	E	270	SER
1	E	281	ILE
1	F	27	ILE
1	F	30	THR
1	F	44	LEU
1	F	50	GLU
1	F	73	ILE
1	F	91	ASN
1	F	102	LYS
1	F	131	VAL
1	F	132	GLU
1	F	147	GLN
1	F	178	THR

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Mol	Chain	Res	Type
1	F	183	ASN
1	F	206	ASP
1	F	218	LEU
1	F	227	MET
1	F	229	LEU
1	F	231	LEU
1	F	268	LEU
1	F	270	SER
1	F	276	GLU
1	F	281	ILE
1	G	27	ILE
1	G	30	THR
1	G	44	LEU
1	G	50	GLU
1	G	73	ILE
1	G	91	ASN
1	G	131	VAL
1	G	147	GLN
1	G	178	THR
1	G	206	ASP
1	G	218	LEU
1	G	227	MET
1	G	229	LEU
1	G	231	LEU
1	G	268	LEU
1	G	270	SER
1	G	276	GLU
1	G	281	ILE
1	H	27	ILE
1	H	30	THR
1	H	44	LEU
1	H	50	GLU
1	H	73	ILE
1	H	91	ASN
1	H	131	VAL
1	H	147	GLN
1	H	178	THR
1	H	206	ASP
1	H	218	LEU
1	H	227	MET
1	H	229	LEU
1	H	231	LEU

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Mol	Chain	Res	Type
1	H	268	LEU
1	H	270	SER
1	H	276	GLU
1	H	281	ILE
1	I	27	ILE
1	I	30	THR
1	I	44	LEU
1	I	50	GLU
1	I	73	ILE
1	I	91	ASN
1	I	131	VAL
1	I	147	GLN
1	I	178	THR
1	I	206	ASP
1	I	218	LEU
1	I	227	MET
1	I	229	LEU
1	I	231	LEU
1	I	270	SER
1	I	276	GLU
1	I	281	ILE
1	J	27	ILE
1	J	30	THR
1	J	44	LEU
1	J	50	GLU
1	J	73	ILE
1	J	91	ASN
1	J	131	VAL
1	J	147	GLN
1	J	178	THR
1	J	206	ASP
1	J	218	LEU
1	J	227	MET
1	J	229	LEU
1	J	231	LEU
1	J	268	LEU
1	J	270	SER
1	J	276	GLU
1	J	281	ILE
1	K	27	ILE
1	K	30	THR
1	K	44	LEU

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Mol	Chain	Res	Type
1	K	50	GLU
1	K	57	LYS
1	K	73	ILE
1	K	91	ASN
1	K	131	VAL
1	K	147	GLN
1	K	178	THR
1	K	206	ASP
1	K	218	LEU
1	K	227	MET
1	K	229	LEU
1	K	231	LEU
1	K	268	LEU
1	K	270	SER
1	K	276	GLU
1	K	281	ILE
1	L	27	ILE
1	L	30	THR
1	L	44	LEU
1	L	50	GLU
1	L	73	ILE
1	L	91	ASN
1	L	131	VAL
1	L	147	GLN
1	L	178	THR
1	L	206	ASP
1	L	218	LEU
1	L	227	MET
1	L	229	LEU
1	L	231	LEU
1	L	268	LEU
1	L	270	SER
1	L	276	GLU
1	L	281	ILE
1	M	27	ILE
1	M	30	THR
1	M	44	LEU
1	M	50	GLU
1	M	73	ILE
1	M	78	TYR
1	M	91	ASN
1	M	131	VAL

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Mol	Chain	Res	Type
1	M	147	GLN
1	M	178	THR
1	M	206	ASP
1	M	218	LEU
1	M	227	MET
1	M	229	LEU
1	M	231	LEU
1	M	268	LEU
1	M	270	SER
1	M	276	GLU
1	M	281	ILE
1	N	27	ILE
1	N	30	THR
1	N	44	LEU
1	N	50	GLU
1	N	73	ILE
1	N	91	ASN
1	N	131	VAL
1	N	147	GLN
1	N	178	THR
1	N	206	ASP
1	N	218	LEU
1	N	227	MET
1	N	229	LEU
1	N	231	LEU
1	N	268	LEU
1	N	270	SER
1	N	276	GLU
1	N	281	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	147	GLN
1	A	256	ASN
1	A	266	ASN
1	B	128	ASN
1	B	147	GLN
1	B	256	ASN
1	B	266	ASN
1	C	128	ASN

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Mol	Chain	Res	Type
1	C	147	GLN
1	C	256	ASN
1	C	266	ASN
1	D	147	GLN
1	D	256	ASN
1	D	266	ASN
1	E	128	ASN
1	E	147	GLN
1	E	256	ASN
1	E	266	ASN
1	F	62	ASN
1	F	128	ASN
1	F	147	GLN
1	F	256	ASN
1	F	266	ASN
1	G	128	ASN
1	G	147	GLN
1	G	256	ASN
1	G	266	ASN
1	H	128	ASN
1	H	256	ASN
1	H	266	ASN
1	I	62	ASN
1	I	128	ASN
1	I	256	ASN
1	I	266	ASN
1	J	53	HIS
1	J	128	ASN
1	J	147	GLN
1	J	256	ASN
1	J	266	ASN
1	K	128	ASN
1	K	147	GLN
1	K	256	ASN
1	K	266	ASN
1	L	128	ASN
1	L	147	GLN
1	L	256	ASN
1	L	266	ASN
1	M	62	ASN
1	M	128	ASN
1	M	147	GLN

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Mol	Chain	Res	Type
1	M	256	ASN
1	M	266	ASN
1	N	128	ASN
1	N	147	GLN
1	N	256	ASN
1	N	266	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](#)

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	267/296 (90%)	1.10	33 (12%) 8 11	3, 61, 120, 283	0
1	B	267/296 (90%)	1.21	48 (17%) 3 6	23, 70, 128, 261	0
1	C	267/296 (90%)	1.29	50 (18%) 3 6	13, 78, 135, 315	0
1	D	267/296 (90%)	1.53	74 (27%) 1 3	28, 89, 137, 213	0
1	E	267/296 (90%)	1.55	79 (29%) 1 3	36, 91, 155, 249	0
1	F	267/296 (90%)	1.49	71 (26%) 1 3	18, 84, 140, 260	0
1	G	267/296 (90%)	1.31	47 (17%) 4 6	18, 70, 131, 170	0
1	H	267/296 (90%)	1.21	42 (15%) 5 8	21, 67, 124, 284	0
1	I	267/296 (90%)	1.34	64 (23%) 2 4	15, 69, 117, 180	0
1	J	267/296 (90%)	1.17	46 (17%) 4 7	6, 67, 114, 214	0
1	K	267/296 (90%)	1.16	48 (17%) 3 6	3, 59, 117, 239	0
1	L	267/296 (90%)	1.15	39 (14%) 6 9	2, 56, 108, 168	0
1	M	267/296 (90%)	1.22	46 (17%) 4 7	9, 59, 114, 292	0
1	N	267/296 (90%)	1.31	49 (18%) 3 6	4, 70, 126, 227	0
All	All	3738/4144 (90%)	1.29	736 (19%) 3 5	2, 71, 132, 315	0

All (736) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	222	GLY	7.9
1	B	222	GLY	7.1
1	A	222	GLY	6.9
1	C	269	SER	5.9
1	N	269	SER	5.9
1	E	269	SER	5.8
1	H	79	TYR	5.6
1	G	222	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	M	113	ASP	5.4
1	K	222	GLY	5.4
1	C	33	ASP	5.2
1	E	136	ALA	5.2
1	C	285	ASP	5.1
1	E	284	GLN	5.1
1	H	136	ALA	5.1
1	K	285	ASP	5.0
1	F	183	ASN	5.0
1	M	269	SER	4.9
1	D	222	GLY	4.9
1	H	148	ASN	4.8
1	N	80	GLY	4.8
1	G	269	SER	4.7
1	G	224	SER	4.7
1	I	100	ASN	4.7
1	J	222	GLY	4.7
1	M	222	GLY	4.7
1	E	285	ASP	4.6
1	F	222	GLY	4.6
1	E	80	GLY	4.6
1	A	194	GLN	4.6
1	K	181	GLY	4.5
1	F	198	LYS	4.5
1	C	222	GLY	4.5
1	M	271	THR	4.4
1	K	202	TYR	4.4
1	B	165	ASP	4.4
1	L	165	ASP	4.4
1	E	222	GLY	4.4
1	C	113	ASP	4.3
1	A	191	TYR	4.3
1	L	100	ASN	4.3
1	F	80	GLY	4.3
1	K	136	ALA	4.2
1	G	64	GLU	4.2
1	F	98	ASN	4.2
1	M	256	ASN	4.2
1	D	96	ASP	4.2
1	J	100	ASN	4.2
1	J	256	ASN	4.2
1	N	222	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	K	274	TYR	4.1
1	D	285	ASP	4.1
1	E	237	ALA	4.1
1	B	285	ASP	4.1
1	K	223	PHE	4.1
1	J	284	GLN	4.0
1	M	25	GLU	4.0
1	K	95	ALA	4.0
1	M	223	PHE	4.0
1	A	256	ASN	4.0
1	C	51	ASP	4.0
1	D	97	VAL	3.9
1	C	57	LYS	3.9
1	N	136	ALA	3.9
1	M	145	ASN	3.9
1	G	43	THR	3.9
1	F	233	ALA	3.9
1	H	269	SER	3.9
1	G	25	GLU	3.9
1	E	266	ASN	3.9
1	D	86	GLU	3.9
1	I	197	MET	3.9
1	H	284	GLN	3.8
1	M	258	GLU	3.8
1	J	269	SER	3.8
1	F	262	TRP	3.7
1	G	223	PHE	3.7
1	N	223	PHE	3.7
1	N	187	TYR	3.7
1	I	194	GLN	3.7
1	I	222	GLY	3.7
1	M	64	GLU	3.7
1	B	284	GLN	3.7
1	I	137	GLY	3.7
1	F	269	SER	3.7
1	G	284	GLN	3.7
1	H	65	GLY	3.7
1	A	258	GLU	3.6
1	H	165	ASP	3.6
1	D	256	ASN	3.6
1	H	74	PHE	3.6
1	E	254	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	166	ALA	3.6
1	L	269	SER	3.6
1	D	101	ILE	3.6
1	D	64	GLU	3.6
1	F	199	SER	3.6
1	J	285	ASP	3.6
1	D	123	TYR	3.5
1	D	257	TRP	3.5
1	I	132	GLU	3.5
1	L	233	ALA	3.5
1	H	98	ASN	3.5
1	D	237	ALA	3.5
1	M	192	GLY	3.5
1	M	285	ASP	3.5
1	E	43	THR	3.5
1	G	122	GLY	3.5
1	C	200	ARG	3.5
1	N	189	ALA	3.5
1	H	30	THR	3.5
1	H	43	THR	3.5
1	B	55	ASP	3.4
1	F	273	GLU	3.4
1	K	74	PHE	3.4
1	D	62	ASN	3.4
1	I	256	ASN	3.4
1	M	43	THR	3.4
1	C	194	GLN	3.4
1	F	208	ASN	3.4
1	A	113	ASP	3.4
1	B	258	GLU	3.4
1	H	100	ASN	3.4
1	C	100	ASN	3.4
1	A	269	SER	3.4
1	F	78	TYR	3.4
1	N	188	HIS	3.4
1	K	237	ALA	3.3
1	D	148	ASN	3.3
1	B	132	GLU	3.3
1	I	286	HIS	3.3
1	E	211	ASP	3.3
1	A	223	PHE	3.3
1	D	145	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	144	TYR	3.3
1	D	29	TYR	3.3
1	J	25	GLU	3.3
1	A	123	TYR	3.3
1	C	68	PRO	3.3
1	I	266	ASN	3.3
1	I	96	ASP	3.3
1	D	65	GLY	3.3
1	F	223	PHE	3.2
1	G	113	ASP	3.2
1	E	32	SER	3.2
1	J	197	MET	3.2
1	F	211	ASP	3.2
1	E	165	ASP	3.2
1	K	256	ASN	3.2
1	C	25	GLU	3.2
1	D	214	ASP	3.2
1	J	51	ASP	3.2
1	I	291	TYR	3.2
1	N	166	ALA	3.2
1	H	54	SER	3.2
1	B	37	HIS	3.2
1	I	65	GLY	3.1
1	C	284	GLN	3.1
1	K	284	GLN	3.1
1	L	226	ASN	3.1
1	F	191	TYR	3.1
1	N	291	TYR	3.1
1	D	142	ALA	3.1
1	E	228	ALA	3.1
1	J	223	PHE	3.1
1	H	194	GLN	3.1
1	C	256	ASN	3.1
1	M	191	TYR	3.1
1	E	132	GLU	3.1
1	B	133	GLY	3.1
1	N	43	THR	3.1
1	E	56	LYS	3.1
1	D	94	SER	3.1
1	M	166	ALA	3.1
1	C	86	GLU	3.1
1	D	184	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	250	ASP	3.1
1	J	80	GLY	3.1
1	D	189	ALA	3.1
1	E	233	ALA	3.1
1	J	86	GLU	3.1
1	F	271	THR	3.1
1	G	147	GLN	3.0
1	E	95	ALA	3.0
1	D	291	TYR	3.0
1	I	148	ASN	3.0
1	I	202	TYR	3.0
1	C	278	MET	3.0
1	J	194	GLN	3.0
1	D	197	MET	3.0
1	F	64	GLU	3.0
1	J	185	ASP	3.0
1	K	211	ASP	3.0
1	I	223	PHE	3.0
1	F	148	ASN	3.0
1	L	64	GLU	3.0
1	M	75	GLY	3.0
1	C	156	ASP	3.0
1	F	149	THR	3.0
1	I	260	THR	3.0
1	E	62	ASN	3.0
1	H	81	LYS	3.0
1	D	223	PHE	3.0
1	D	261	GLN	3.0
1	I	36	SER	3.0
1	E	281	ILE	2.9
1	M	101	ILE	2.9
1	E	60	LEU	2.9
1	G	46	GLY	2.9
1	I	269	SER	2.9
1	B	286	HIS	2.9
1	E	81	LYS	2.9
1	G	286	HIS	2.9
1	F	282	ASN	2.9
1	M	100	ASN	2.9
1	I	258	GLU	2.9
1	E	45	SER	2.9
1	G	36	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	165	ASP	2.9
1	F	177	GLU	2.9
1	G	257	TRP	2.9
1	E	97	VAL	2.9
1	M	194	GLN	2.9
1	F	71	LYS	2.9
1	J	71	LYS	2.9
1	B	223	PHE	2.9
1	L	285	ASP	2.9
1	A	62	ASN	2.9
1	J	64	GLU	2.9
1	A	80	GLY	2.9
1	H	198	LYS	2.9
1	L	179	LYS	2.9
1	J	26	ALA	2.9
1	D	209	PHE	2.9
1	F	209	PHE	2.9
1	L	202	TYR	2.9
1	C	37	HIS	2.9
1	N	91	ASN	2.9
1	F	241	VAL	2.9
1	F	48	PHE	2.9
1	D	182	TYR	2.9
1	H	191	TYR	2.9
1	E	251	ASN	2.9
1	K	273	GLU	2.9
1	N	177	GLU	2.9
1	D	224	SER	2.8
1	L	36	SER	2.8
1	F	46	GLY	2.8
1	E	166	ALA	2.8
1	D	191	TYR	2.8
1	J	198	LYS	2.8
1	D	204	ASN	2.8
1	F	132	GLU	2.8
1	N	165	ASP	2.8
1	D	95	ALA	2.8
1	D	233	ALA	2.8
1	E	223	PHE	2.8
1	M	198	LYS	2.8
1	N	29	TYR	2.8
1	N	64	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	167	ASN	2.8
1	F	181	GLY	2.8
1	D	165	ASP	2.8
1	N	156	ASP	2.8
1	B	269	SER	2.8
1	H	25	GLU	2.8
1	K	204	ASN	2.8
1	L	74	PHE	2.8
1	F	55	ASP	2.8
1	I	165	ASP	2.8
1	K	134	LYS	2.8
1	M	32	SER	2.8
1	B	145	ASN	2.8
1	L	145	ASN	2.8
1	N	65	GLY	2.8
1	C	237	ALA	2.8
1	G	201	LEU	2.8
1	D	32	SER	2.8
1	B	29	TYR	2.8
1	I	182	TYR	2.8
1	M	205	GLY	2.8
1	G	98	ASN	2.8
1	F	259	THR	2.8
1	B	79	TYR	2.7
1	D	284	GLN	2.7
1	C	43	THR	2.7
1	G	217	THR	2.7
1	N	109	LYS	2.7
1	K	80	GLY	2.7
1	M	29	TYR	2.7
1	M	79	TYR	2.7
1	J	273	GLU	2.7
1	C	145	ASN	2.7
1	D	100	ASN	2.7
1	E	141	ASN	2.7
1	E	260	THR	2.7
1	F	193	ASN	2.7
1	L	30	THR	2.7
1	M	148	ASN	2.7
1	C	286	HIS	2.7
1	G	136	ALA	2.7
1	E	64	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	224	SER	2.7
1	C	291	TYR	2.7
1	F	291	TYR	2.7
1	A	220	SER	2.7
1	E	240	SER	2.7
1	B	80	GLY	2.7
1	I	101	ILE	2.7
1	K	29	TYR	2.7
1	L	80	GLY	2.7
1	M	254	ILE	2.7
1	J	79	TYR	2.7
1	N	123	TYR	2.7
1	A	86	GLU	2.7
1	B	25	GLU	2.7
1	I	149	THR	2.7
1	M	132	GLU	2.7
1	M	260	THR	2.7
1	I	193	ASN	2.7
1	N	266	ASN	2.7
1	N	37	HIS	2.6
1	E	84	TRP	2.6
1	E	252	ASP	2.6
1	L	290	TYR	2.6
1	B	30	THR	2.6
1	E	259	THR	2.6
1	J	77	LYS	2.6
1	K	289	GLU	2.6
1	A	145	ASN	2.6
1	B	148	ASN	2.6
1	E	85	PRO	2.6
1	B	181	GLY	2.6
1	H	133	GLY	2.6
1	L	133	GLY	2.6
1	B	152	TYR	2.6
1	F	159	THR	2.6
1	F	182	TYR	2.6
1	I	30	THR	2.6
1	F	258	GLU	2.6
1	H	197	MET	2.6
1	N	153	GLU	2.6
1	D	143	SER	2.6
1	I	76	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	56	LYS	2.6
1	L	194	GLN	2.6
1	D	271	THR	2.6
1	E	246	TYR	2.6
1	H	33	ASP	2.6
1	E	275	ASN	2.6
1	I	98	ASN	2.6
1	M	98	ASN	2.6
1	N	100	ASN	2.6
1	N	288	ILE	2.6
1	E	52	PRO	2.6
1	L	237	ALA	2.6
1	N	39	GLY	2.6
1	A	29	TYR	2.6
1	E	40	TRP	2.6
1	E	291	TYR	2.6
1	G	70	ASP	2.6
1	F	105	ASN	2.6
1	I	47	THR	2.6
1	M	187	TYR	2.6
1	L	50	GLU	2.6
1	K	54	SER	2.6
1	B	263	ARG	2.6
1	A	147	GLN	2.6
1	D	135	THR	2.5
1	G	58	THR	2.5
1	F	140	ILE	2.5
1	B	162	ARG	2.5
1	L	25	GLU	2.5
1	L	131	VAL	2.5
1	K	165	ASP	2.5
1	F	124	SER	2.5
1	G	132	GLU	2.5
1	I	68	PRO	2.5
1	E	198	LYS	2.5
1	K	198	LYS	2.5
1	E	149	THR	2.5
1	B	191	TYR	2.5
1	G	120	SER	2.5
1	A	96	ASP	2.5
1	E	164	ASP	2.5
1	F	285	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	285	ASP	2.5
1	G	71	LYS	2.5
1	L	56	LYS	2.5
1	D	149	THR	2.5
1	I	43	THR	2.5
1	C	272	SER	2.5
1	D	231	LEU	2.5
1	C	258	GLU	2.5
1	C	261	GLN	2.5
1	D	219	ILE	2.5
1	G	237	ALA	2.5
1	J	235	LYS	2.5
1	I	82	MET	2.5
1	H	223	PHE	2.5
1	I	40	TRP	2.5
1	F	57	LYS	2.5
1	G	154	GLN	2.5
1	N	142	ALA	2.5
1	B	252	ASP	2.5
1	E	156	ASP	2.5
1	I	214	ASP	2.5
1	G	29	TYR	2.5
1	H	132	GLU	2.4
1	K	25	GLU	2.4
1	D	281	ILE	2.4
1	F	40	TRP	2.4
1	F	101	ILE	2.4
1	L	148	ASN	2.4
1	E	255	LEU	2.4
1	K	122	GLY	2.4
1	B	185	ASP	2.4
1	I	250	ASP	2.4
1	L	172	ASP	2.4
1	D	198	LYS	2.4
1	J	207	LYS	2.4
1	A	254	ILE	2.4
1	J	167	ASN	2.4
1	N	98	ASN	2.4
1	I	192	GLY	2.4
1	J	65	GLY	2.4
1	L	222	GLY	2.4
1	B	143	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	32	SER	2.4
1	F	214	ASP	2.4
1	F	250	ASP	2.4
1	G	214	ASP	2.4
1	K	87	THR	2.4
1	D	74	PHE	2.4
1	B	291	TYR	2.4
1	E	29	TYR	2.4
1	G	291	TYR	2.4
1	A	237	ALA	2.4
1	G	189	ALA	2.4
1	F	256	ASN	2.4
1	J	271	THR	2.4
1	C	29	TYR	2.4
1	A	95	ALA	2.4
1	F	237	ALA	2.4
1	J	83	LYS	2.4
1	M	140	ILE	2.4
1	H	113	ASP	2.4
1	L	206	ASP	2.4
1	N	33	ASP	2.4
1	N	273	GLU	2.4
1	E	283	TRP	2.4
1	H	192	GLY	2.4
1	J	148	ASN	2.4
1	N	58	THR	2.4
1	C	44	LEU	2.4
1	C	142	ALA	2.4
1	G	153	GLU	2.4
1	G	235	LYS	2.4
1	J	37	HIS	2.3
1	D	203	ASN	2.3
1	E	100	ASN	2.3
1	F	62	ASN	2.3
1	I	99	ASN	2.3
1	D	103	ILE	2.3
1	E	232	THR	2.3
1	N	263	ARG	2.3
1	F	82	MET	2.3
1	F	172	ASP	2.3
1	H	180	ASP	2.3
1	N	164	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	166	ALA	2.3
1	A	143	SER	2.3
1	B	124	SER	2.3
1	D	121	ILE	2.3
1	K	68	PRO	2.3
1	A	266	ASN	2.3
1	J	98	ASN	2.3
1	C	93	LYS	2.3
1	E	289	GLU	2.3
1	G	194	GLN	2.3
1	G	289	GLU	2.3
1	I	33	ASP	2.3
1	M	177	GLU	2.3
1	E	103	ILE	2.3
1	F	67	ILE	2.3
1	A	65	GLY	2.3
1	D	122	GLY	2.3
1	I	126	GLY	2.3
1	N	120	SER	2.3
1	N	128	ASN	2.3
1	F	200	ARG	2.3
1	I	213	ARG	2.3
1	K	278	MET	2.3
1	B	64	GLU	2.3
1	D	33	ASP	2.3
1	F	70	ASP	2.3
1	I	86	GLU	2.3
1	B	45	SER	2.3
1	I	75	GLY	2.3
1	N	192	GLY	2.3
1	F	167	ASN	2.3
1	L	167	ASN	2.3
1	N	257	TRP	2.3
1	E	67	ILE	2.3
1	E	101	ILE	2.3
1	F	29	TYR	2.3
1	K	291	TYR	2.3
1	B	194	GLN	2.3
1	H	199	SER	2.3
1	H	270	SER	2.3
1	L	220	SER	2.3
1	I	264	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	96	ASP	2.3
1	K	116	ASP	2.3
1	D	77	LYS	2.3
1	D	200	ARG	2.3
1	I	128	ASN	2.3
1	K	203	ASN	2.3
1	J	67	ILE	2.3
1	K	194	GLN	2.3
1	B	32	SER	2.3
1	G	50	GLU	2.3
1	L	94	SER	2.3
1	B	198	LYS	2.3
1	E	214	ASP	2.3
1	F	156	ASP	2.3
1	J	30	THR	2.2
1	K	62	ASN	2.2
1	B	168	LEU	2.2
1	G	268	LEU	2.2
1	N	40	TRP	2.2
1	F	254	ILE	2.2
1	I	142	ALA	2.2
1	F	79	TYR	2.2
1	F	284	GLN	2.2
1	I	29	TYR	2.2
1	K	144	TYR	2.2
1	N	284	GLN	2.2
1	F	83	LYS	2.2
1	I	32	SER	2.2
1	K	45	SER	2.2
1	C	34	THR	2.2
1	M	217	THR	2.2
1	A	148	ASN	2.2
1	C	236	ASN	2.2
1	D	282	ASN	2.2
1	D	48	PHE	2.2
1	F	90	ILE	2.2
1	F	36	SER	2.2
1	K	78	TYR	2.2
1	D	278	MET	2.2
1	A	276	GLU	2.2
1	E	258	GLU	2.2
1	I	25	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	25	GLU	2.2
1	E	122	GLY	2.2
1	B	271	THR	2.2
1	I	259	THR	2.2
1	M	188	HIS	2.2
1	D	83	LYS	2.2
1	E	262	TRP	2.2
1	F	84	TRP	2.2
1	A	45	SER	2.2
1	B	197	MET	2.2
1	C	290	TYR	2.2
1	D	39	GLY	2.2
1	E	245	GLU	2.2
1	D	225	PRO	2.2
1	E	30	THR	2.2
1	I	203	ASN	2.2
1	L	91	ASN	2.2
1	L	204	ASN	2.2
1	F	134	LYS	2.2
1	M	237	ALA	2.2
1	I	143	SER	2.2
1	A	79	TYR	2.2
1	J	202	TYR	2.2
1	K	187	TYR	2.2
1	D	276	GLU	2.2
1	N	50	GLU	2.2
1	C	101	ILE	2.2
1	H	265	THR	2.2
1	N	259	THR	2.2
1	M	77	LYS	2.2
1	F	203	ASN	2.2
1	G	204	ASN	2.2
1	J	53	HIS	2.2
1	J	166	ALA	2.2
1	F	154	GLN	2.2
1	E	88	TYR	2.2
1	E	241	VAL	2.2
1	H	290	TYR	2.2
1	B	137	GLY	2.2
1	H	67	ILE	2.2
1	J	177	GLU	2.2
1	F	81	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	179	LYS	2.2
1	I	62	ASN	2.2
1	D	255	LEU	2.2
1	M	197	MET	2.2
1	A	263	ARG	2.1
1	E	263	ARG	2.1
1	H	51	ASP	2.1
1	I	51	ASP	2.1
1	J	116	ASP	2.1
1	L	76	SER	2.1
1	M	224	SER	2.1
1	N	252	ASP	2.1
1	L	147	GLN	2.1
1	E	78	TYR	2.1
1	E	274	TYR	2.1
1	B	68	PRO	2.1
1	E	46	GLY	2.1
1	E	83	LYS	2.1
1	I	133	GLY	2.1
1	I	134	LYS	2.1
1	L	149	THR	2.1
1	J	82	MET	2.1
1	C	169	ALA	2.1
1	E	98	ASN	2.1
1	B	154	GLN	2.1
1	I	31	SER	2.1
1	K	147	GLN	2.1
1	A	285	ASP	2.1
1	E	96	ASP	2.1
1	G	172	ASP	2.1
1	G	190	ILE	2.1
1	M	40	TRP	2.1
1	C	191	TYR	2.1
1	C	202	TYR	2.1
1	E	71	LYS	2.1
1	E	79	TYR	2.1
1	J	29	TYR	2.1
1	M	78	TYR	2.1
1	D	221	GLY	2.1
1	A	273	GLU	2.1
1	K	271	THR	2.1
1	B	136	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	233	ALA	2.1
1	H	204	ASN	2.1
1	I	145	ASN	2.1
1	C	118	SER	2.1
1	C	147	GLN	2.1
1	E	194	GLN	2.1
1	N	247	GLN	2.1
1	N	261	GLN	2.1
1	A	198	LYS	2.1
1	C	102	LYS	2.1
1	D	57	LYS	2.1
1	E	209	PHE	2.1
1	G	81	LYS	2.1
1	G	209	PHE	2.1
1	K	109	LYS	2.1
1	J	68	PRO	2.1
1	D	201	LEU	2.1
1	H	149	THR	2.1
1	J	263	ARG	2.1
1	H	189	ALA	2.1
1	D	269	SER	2.1
1	E	69	SER	2.1
1	G	128	ASN	2.1
1	K	167	ASN	2.1
1	D	147	GLN	2.1
1	M	284	GLN	2.1
1	J	209	PHE	2.1
1	M	286	HIS	2.1
1	B	164	ASP	2.1
1	H	214	ASP	2.1
1	B	39	GLY	2.1
1	L	29	TYR	2.1
1	K	64	GLU	2.1
1	G	49	ILE	2.1
1	N	199	SER	2.1
1	B	247	GLN	2.1
1	D	251	ASN	2.1
1	M	268	LEU	2.1
1	M	80	GLY	2.1
1	N	181	GLY	2.1
1	C	132	GLU	2.1
1	E	25	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	109	LYS	2.1
1	L	101	ILE	2.1
1	C	32	SER	2.1
1	C	143	SER	2.1
1	B	65	GLY	2.0
1	C	182	TYR	2.0
1	F	37	HIS	2.0
1	G	165	ASP	2.0
1	F	239	GLU	2.0
1	H	178	THR	2.0
1	H	210	THR	2.0
1	I	172	ASP	2.0
1	I	252	ASP	2.0
1	K	207	LYS	2.0
1	D	66	PHE	2.0
1	G	272	SER	2.0
1	H	45	SER	2.0
1	I	224	SER	2.0
1	D	268	LEU	2.0
1	C	105	ASN	2.0
1	G	82	MET	2.0
1	A	192	GLY	2.0
1	I	181	GLY	2.0
1	E	191	TYR	2.0
1	A	67	ILE	2.0
1	B	67	ILE	2.0
1	G	135	THR	2.0
1	J	34	THR	2.0
1	E	86	GLU	2.0
1	I	70	ASP	2.0
1	K	55	ASP	2.0
1	B	272	SER	2.0
1	C	36	SER	2.0
1	C	209	PHE	2.0
1	H	230	ALA	2.0
1	I	196	PHE	2.0
1	K	120	SER	2.0
1	D	226	ASN	2.0
1	D	181	GLY	2.0
1	E	179	LYS	2.0
1	K	65	GLY	2.0
1	D	155	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	254	ILE	2.0
1	I	191	TYR	2.0
1	I	288	ILE	2.0
1	L	79	TYR	2.0
1	M	291	TYR	2.0
1	N	202	TYR	2.0
1	J	43	THR	2.0
1	K	40	TRP	2.0
1	L	177	GLU	2.0
1	D	136	ALA	2.0
1	K	270	SER	2.0
1	L	45	SER	2.0
1	M	270	SER	2.0
1	C	241	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.