Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2020 – 12:52 pm BST

PDB ID	:	6RIM
Title	:	Crystal structure of the catalytic domain of the Weissela oryzae botulinum like toxin
Authors	:	Kosenina, S.; Masuyer, G.; Stenmark, P.
Deposited on	:	2019-04-24
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

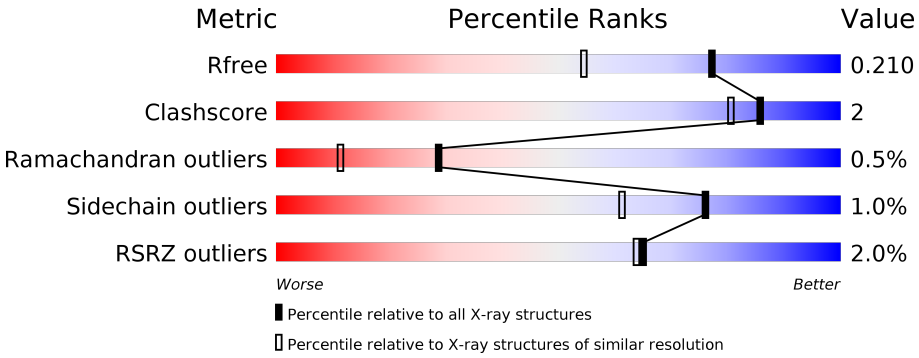
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	498	2% 85% • 11%
1	B	498	2% 86% • 11%
1	C	498	3% 82% 5% • 12%
1	D	498	2% 84% • 12%
1	E	498	3% 84% 7% • 8%
1	F	498	87% • • 8%

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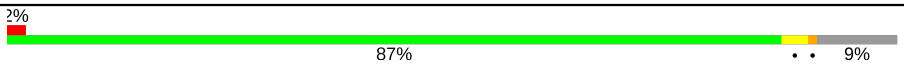
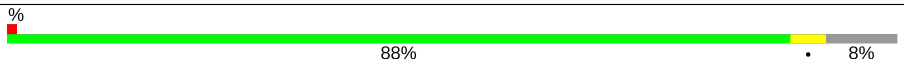
Mol	Chain	Length	Quality of chain
1	G	498	
1	H	498	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32682 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 Putative botulinum-like toxin Wo.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	Se	0	3	0
			3595	2284	595	706	4	6			
1	B	442	Total	C	N	O	S	Se	0	2	0
			3595	2289	590	705	4	7			
1	C	440	Total	C	N	O	S	Se	0	4	0
			3594	2284	590	710	4	6			
1	D	439	Total	C	N	O	S	Se	0	4	0
			3588	2283	588	705	5	7			
1	E	457	Total	C	N	O	S	Se	0	6	0
			3736	2370	615	740	4	7			
1	F	458	Total	C	N	O	S	Se	0	5	0
			3733	2367	614	740	5	7			
1	G	451	Total	C	N	O	S	Se	0	5	0
			3682	2338	606	727	4	7			
1	H	458	Total	C	N	O	S	Se	0	4	0
			3730	2367	614	737	5	7			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	initiating methionine	UNP A0A069CUU9
A	-20	GLY	-	expression tag	UNP A0A069CUU9
A	-19	SER	-	expression tag	UNP A0A069CUU9
A	-18	SER	-	expression tag	UNP A0A069CUU9
A	-17	HIS	-	expression tag	UNP A0A069CUU9
A	-16	HIS	-	expression tag	UNP A0A069CUU9
A	-15	HIS	-	expression tag	UNP A0A069CUU9
A	-14	HIS	-	expression tag	UNP A0A069CUU9
A	-13	HIS	-	expression tag	UNP A0A069CUU9
A	-12	HIS	-	expression tag	UNP A0A069CUU9
A	-11	SER	-	expression tag	UNP A0A069CUU9
A	-10	SER	-	expression tag	UNP A0A069CUU9
A	-9	GLY	-	expression tag	UNP A0A069CUU9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	LEU	-	expression tag	UNP A0A069CUU9
A	-7	VAL	-	expression tag	UNP A0A069CUU9
A	-6	PRO	-	expression tag	UNP A0A069CUU9
A	-5	ARG	-	expression tag	UNP A0A069CUU9
A	-4	GLY	-	expression tag	UNP A0A069CUU9
A	-3	SER	-	expression tag	UNP A0A069CUU9
A	-2	HIS	-	expression tag	UNP A0A069CUU9
A	-1	MSE	-	expression tag	UNP A0A069CUU9
A	0	ALA	-	expression tag	UNP A0A069CUU9
A	1	SER	-	expression tag	UNP A0A069CUU9
B	-21	MSE	-	initiating methionine	UNP A0A069CUU9
B	-20	GLY	-	expression tag	UNP A0A069CUU9
B	-19	SER	-	expression tag	UNP A0A069CUU9
B	-18	SER	-	expression tag	UNP A0A069CUU9
B	-17	HIS	-	expression tag	UNP A0A069CUU9
B	-16	HIS	-	expression tag	UNP A0A069CUU9
B	-15	HIS	-	expression tag	UNP A0A069CUU9
B	-14	HIS	-	expression tag	UNP A0A069CUU9
B	-13	HIS	-	expression tag	UNP A0A069CUU9
B	-12	HIS	-	expression tag	UNP A0A069CUU9
B	-11	SER	-	expression tag	UNP A0A069CUU9
B	-10	SER	-	expression tag	UNP A0A069CUU9
B	-9	GLY	-	expression tag	UNP A0A069CUU9
B	-8	LEU	-	expression tag	UNP A0A069CUU9
B	-7	VAL	-	expression tag	UNP A0A069CUU9
B	-6	PRO	-	expression tag	UNP A0A069CUU9
B	-5	ARG	-	expression tag	UNP A0A069CUU9
B	-4	GLY	-	expression tag	UNP A0A069CUU9
B	-3	SER	-	expression tag	UNP A0A069CUU9
B	-2	HIS	-	expression tag	UNP A0A069CUU9
B	-1	MSE	-	expression tag	UNP A0A069CUU9
B	0	ALA	-	expression tag	UNP A0A069CUU9
B	1	SER	-	expression tag	UNP A0A069CUU9
C	-21	MSE	-	initiating methionine	UNP A0A069CUU9
C	-20	GLY	-	expression tag	UNP A0A069CUU9
C	-19	SER	-	expression tag	UNP A0A069CUU9
C	-18	SER	-	expression tag	UNP A0A069CUU9
C	-17	HIS	-	expression tag	UNP A0A069CUU9
C	-16	HIS	-	expression tag	UNP A0A069CUU9
C	-15	HIS	-	expression tag	UNP A0A069CUU9
C	-14	HIS	-	expression tag	UNP A0A069CUU9
C	-13	HIS	-	expression tag	UNP A0A069CUU9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP A0A069CUU9
C	-11	SER	-	expression tag	UNP A0A069CUU9
C	-10	SER	-	expression tag	UNP A0A069CUU9
C	-9	GLY	-	expression tag	UNP A0A069CUU9
C	-8	LEU	-	expression tag	UNP A0A069CUU9
C	-7	VAL	-	expression tag	UNP A0A069CUU9
C	-6	PRO	-	expression tag	UNP A0A069CUU9
C	-5	ARG	-	expression tag	UNP A0A069CUU9
C	-4	GLY	-	expression tag	UNP A0A069CUU9
C	-3	SER	-	expression tag	UNP A0A069CUU9
C	-2	HIS	-	expression tag	UNP A0A069CUU9
C	-1	MSE	-	expression tag	UNP A0A069CUU9
C	0	ALA	-	expression tag	UNP A0A069CUU9
C	1	SER	-	expression tag	UNP A0A069CUU9
D	-21	MSE	-	initiating methionine	UNP A0A069CUU9
D	-20	GLY	-	expression tag	UNP A0A069CUU9
D	-19	SER	-	expression tag	UNP A0A069CUU9
D	-18	SER	-	expression tag	UNP A0A069CUU9
D	-17	HIS	-	expression tag	UNP A0A069CUU9
D	-16	HIS	-	expression tag	UNP A0A069CUU9
D	-15	HIS	-	expression tag	UNP A0A069CUU9
D	-14	HIS	-	expression tag	UNP A0A069CUU9
D	-13	HIS	-	expression tag	UNP A0A069CUU9
D	-12	HIS	-	expression tag	UNP A0A069CUU9
D	-11	SER	-	expression tag	UNP A0A069CUU9
D	-10	SER	-	expression tag	UNP A0A069CUU9
D	-9	GLY	-	expression tag	UNP A0A069CUU9
D	-8	LEU	-	expression tag	UNP A0A069CUU9
D	-7	VAL	-	expression tag	UNP A0A069CUU9
D	-6	PRO	-	expression tag	UNP A0A069CUU9
D	-5	ARG	-	expression tag	UNP A0A069CUU9
D	-4	GLY	-	expression tag	UNP A0A069CUU9
D	-3	SER	-	expression tag	UNP A0A069CUU9
D	-2	HIS	-	expression tag	UNP A0A069CUU9
D	-1	MSE	-	expression tag	UNP A0A069CUU9
D	0	ALA	-	expression tag	UNP A0A069CUU9
D	1	SER	-	expression tag	UNP A0A069CUU9
E	-21	MSE	-	initiating methionine	UNP A0A069CUU9
E	-20	GLY	-	expression tag	UNP A0A069CUU9
E	-19	SER	-	expression tag	UNP A0A069CUU9
E	-18	SER	-	expression tag	UNP A0A069CUU9
E	-17	HIS	-	expression tag	UNP A0A069CUU9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	HIS	-	expression tag	UNP A0A069CUU9
E	-15	HIS	-	expression tag	UNP A0A069CUU9
E	-14	HIS	-	expression tag	UNP A0A069CUU9
E	-13	HIS	-	expression tag	UNP A0A069CUU9
E	-12	HIS	-	expression tag	UNP A0A069CUU9
E	-11	SER	-	expression tag	UNP A0A069CUU9
E	-10	SER	-	expression tag	UNP A0A069CUU9
E	-9	GLY	-	expression tag	UNP A0A069CUU9
E	-8	LEU	-	expression tag	UNP A0A069CUU9
E	-7	VAL	-	expression tag	UNP A0A069CUU9
E	-6	PRO	-	expression tag	UNP A0A069CUU9
E	-5	ARG	-	expression tag	UNP A0A069CUU9
E	-4	GLY	-	expression tag	UNP A0A069CUU9
E	-3	SER	-	expression tag	UNP A0A069CUU9
E	-2	HIS	-	expression tag	UNP A0A069CUU9
E	-1	MSE	-	expression tag	UNP A0A069CUU9
E	0	ALA	-	expression tag	UNP A0A069CUU9
E	1	SER	-	expression tag	UNP A0A069CUU9
F	-21	MSE	-	initiating methionine	UNP A0A069CUU9
F	-20	GLY	-	expression tag	UNP A0A069CUU9
F	-19	SER	-	expression tag	UNP A0A069CUU9
F	-18	SER	-	expression tag	UNP A0A069CUU9
F	-17	HIS	-	expression tag	UNP A0A069CUU9
F	-16	HIS	-	expression tag	UNP A0A069CUU9
F	-15	HIS	-	expression tag	UNP A0A069CUU9
F	-14	HIS	-	expression tag	UNP A0A069CUU9
F	-13	HIS	-	expression tag	UNP A0A069CUU9
F	-12	HIS	-	expression tag	UNP A0A069CUU9
F	-11	SER	-	expression tag	UNP A0A069CUU9
F	-10	SER	-	expression tag	UNP A0A069CUU9
F	-9	GLY	-	expression tag	UNP A0A069CUU9
F	-8	LEU	-	expression tag	UNP A0A069CUU9
F	-7	VAL	-	expression tag	UNP A0A069CUU9
F	-6	PRO	-	expression tag	UNP A0A069CUU9
F	-5	ARG	-	expression tag	UNP A0A069CUU9
F	-4	GLY	-	expression tag	UNP A0A069CUU9
F	-3	SER	-	expression tag	UNP A0A069CUU9
F	-2	HIS	-	expression tag	UNP A0A069CUU9
F	-1	MSE	-	expression tag	UNP A0A069CUU9
F	0	ALA	-	expression tag	UNP A0A069CUU9
F	1	SER	-	expression tag	UNP A0A069CUU9
G	-21	MSE	-	initiating methionine	UNP A0A069CUU9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	GLY	-	expression tag	UNP A0A069CUU9
G	-19	SER	-	expression tag	UNP A0A069CUU9
G	-18	SER	-	expression tag	UNP A0A069CUU9
G	-17	HIS	-	expression tag	UNP A0A069CUU9
G	-16	HIS	-	expression tag	UNP A0A069CUU9
G	-15	HIS	-	expression tag	UNP A0A069CUU9
G	-14	HIS	-	expression tag	UNP A0A069CUU9
G	-13	HIS	-	expression tag	UNP A0A069CUU9
G	-12	HIS	-	expression tag	UNP A0A069CUU9
G	-11	SER	-	expression tag	UNP A0A069CUU9
G	-10	SER	-	expression tag	UNP A0A069CUU9
G	-9	GLY	-	expression tag	UNP A0A069CUU9
G	-8	LEU	-	expression tag	UNP A0A069CUU9
G	-7	VAL	-	expression tag	UNP A0A069CUU9
G	-6	PRO	-	expression tag	UNP A0A069CUU9
G	-5	ARG	-	expression tag	UNP A0A069CUU9
G	-4	GLY	-	expression tag	UNP A0A069CUU9
G	-3	SER	-	expression tag	UNP A0A069CUU9
G	-2	HIS	-	expression tag	UNP A0A069CUU9
G	-1	MSE	-	expression tag	UNP A0A069CUU9
G	0	ALA	-	expression tag	UNP A0A069CUU9
G	1	SER	-	expression tag	UNP A0A069CUU9
H	-21	MSE	-	initiating methionine	UNP A0A069CUU9
H	-20	GLY	-	expression tag	UNP A0A069CUU9
H	-19	SER	-	expression tag	UNP A0A069CUU9
H	-18	SER	-	expression tag	UNP A0A069CUU9
H	-17	HIS	-	expression tag	UNP A0A069CUU9
H	-16	HIS	-	expression tag	UNP A0A069CUU9
H	-15	HIS	-	expression tag	UNP A0A069CUU9
H	-14	HIS	-	expression tag	UNP A0A069CUU9
H	-13	HIS	-	expression tag	UNP A0A069CUU9
H	-12	HIS	-	expression tag	UNP A0A069CUU9
H	-11	SER	-	expression tag	UNP A0A069CUU9
H	-10	SER	-	expression tag	UNP A0A069CUU9
H	-9	GLY	-	expression tag	UNP A0A069CUU9
H	-8	LEU	-	expression tag	UNP A0A069CUU9
H	-7	VAL	-	expression tag	UNP A0A069CUU9
H	-6	PRO	-	expression tag	UNP A0A069CUU9
H	-5	ARG	-	expression tag	UNP A0A069CUU9
H	-4	GLY	-	expression tag	UNP A0A069CUU9
H	-3	SER	-	expression tag	UNP A0A069CUU9
H	-2	HIS	-	expression tag	UNP A0A069CUU9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	MSE	-	expression tag	UNP A0A069CUU9
H	0	ALA	-	expression tag	UNP A0A069CUU9
H	1	SER	-	expression tag	UNP A0A069CUU9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is water.

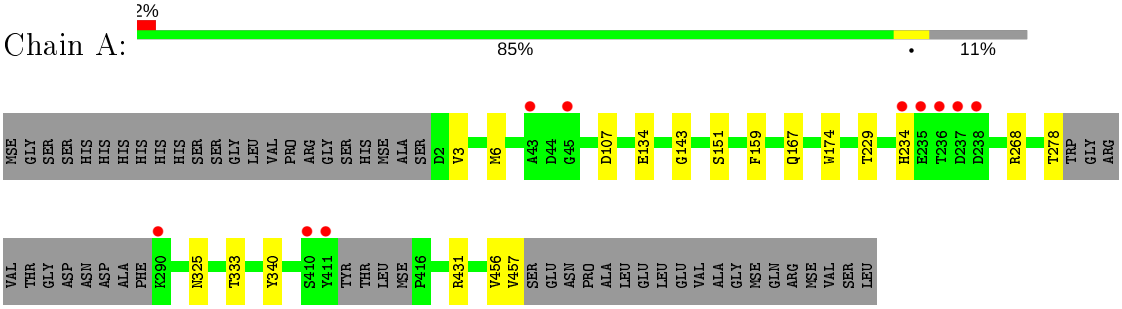
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	441	Total O 441 441	0	0
4	B	395	Total O 395 395	0	0
4	C	431	Total O 431 431	0	0
4	D	389	Total O 389 389	0	0
4	E	455	Total O 455 455	0	0
4	F	426	Total O 426 426	0	0
4	G	456	Total O 456 456	0	0
4	H	420	Total O 420 420	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

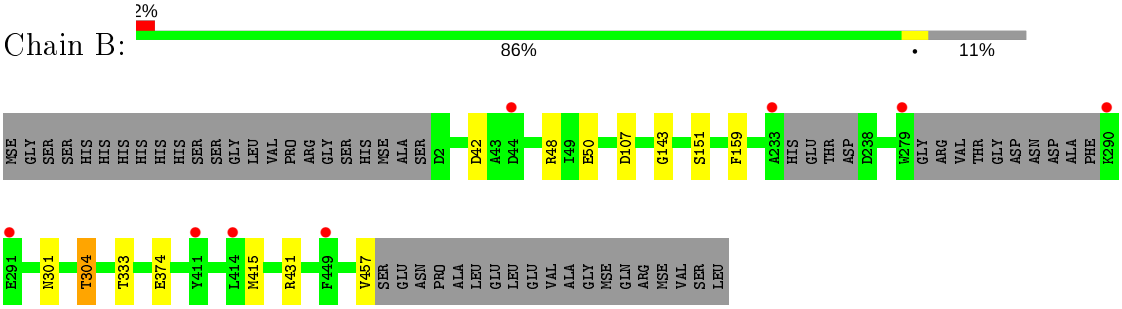
- Molecule 1: Putative botulinum-like toxin Wo

Chain A:



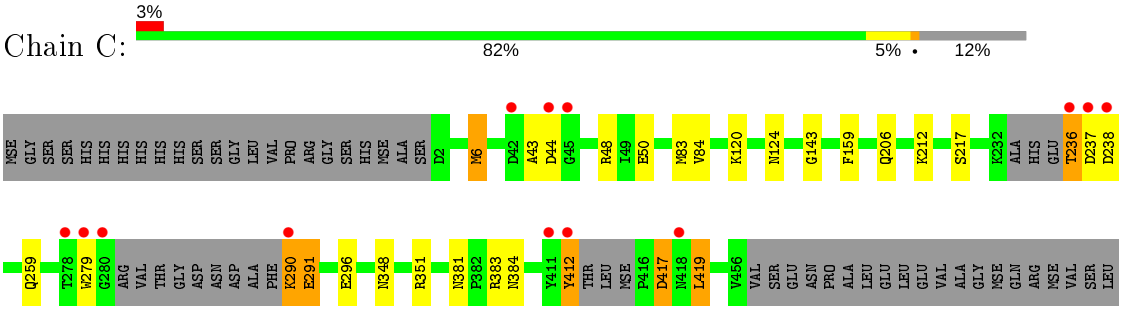
- Molecule 1: Putative botulinum-like toxin Wo

Chain B:



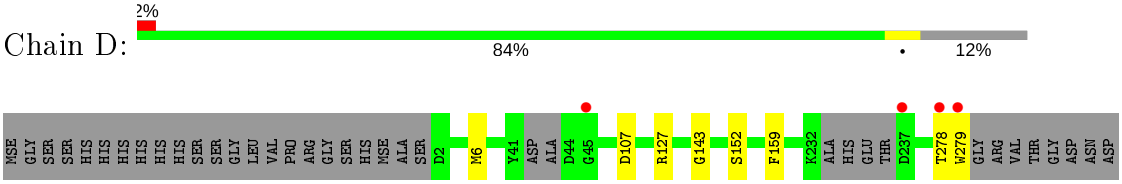
- Molecule 1: Putative botulinum-like toxin Wo

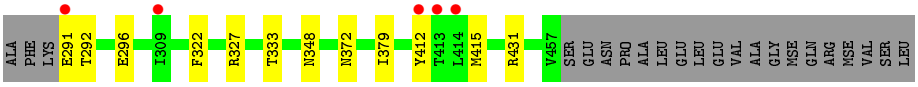
Chain C:



- Molecule 1: Putative botulinum-like toxin Wo

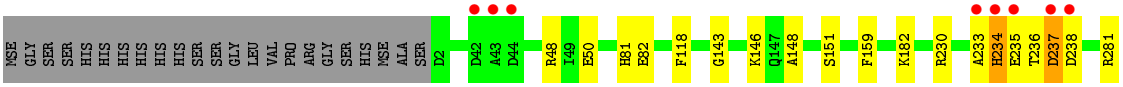
Chain D:

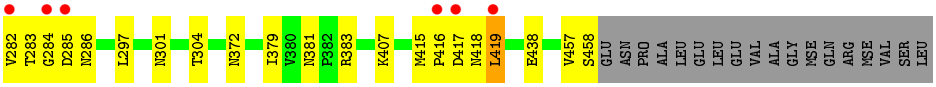




- Molecule 1: Putative botulinum-like toxin Wo

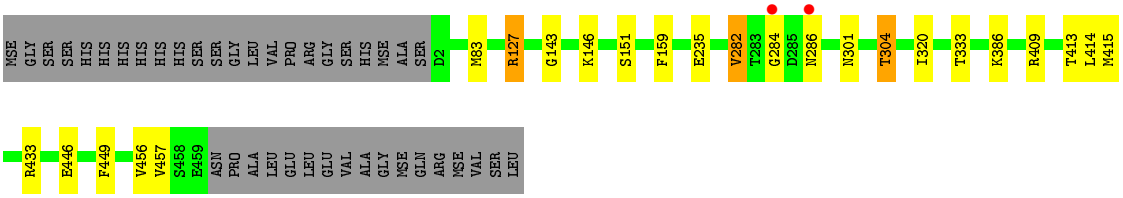
Chain E:





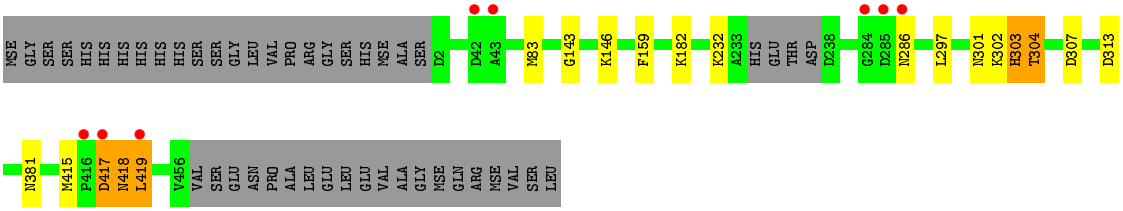
- Molecule 1: Putative botulinum-like toxin Wo

Chain F:



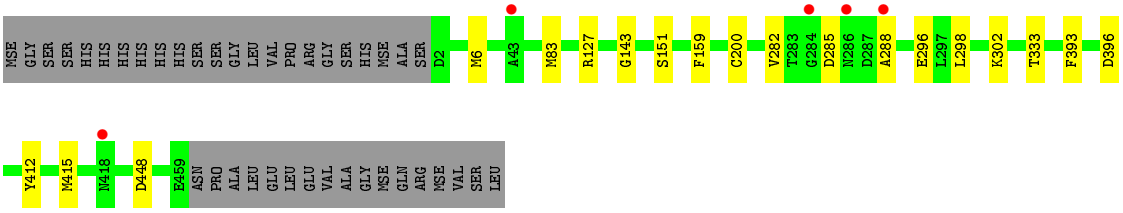
- Molecule 1: Putative botulinum-like toxin Wo

Chain G:



- Molecule 1: Putative botulinum-like toxin Wo

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.91Å 105.21Å 179.62Å 101.71° 90.00° 90.00°	Depositor
Resolution (Å)	58.63 – 1.60 58.63 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (58.63-1.60) 97.0 (58.63-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.151 , 0.202 0.161 , 0.210	Depositor DCC
R_{free} test set	26604 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 29.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	32682	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, CA

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	0.67	0/3672	0.75	1/4953 (0.0%)
1	B	0.66	0/3673	0.73	1/4958 (0.0%)
1	C	0.67	0/3672	0.76	1/4955 (0.0%)
1	D	0.66	0/3665	0.74	2/4946 (0.0%)
1	E	0.69	0/3818	0.77	0/5156
1	F	0.66	0/3815	0.74	2/5153 (0.0%)
1	G	0.70	0/3762	0.76	2/5079 (0.0%)
1	H	0.66	0/3812	0.73	2/5148 (0.0%)
All	All	0.67	0/29889	0.75	11/40348 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	415	MSE	CG-SE-CE	6.81	113.89	98.90
1	F	415	MSE	CG-SE-CE	6.18	112.49	98.90
1	C	6	MSE	CG-SE-CE	-6.05	85.58	98.90
1	B	415	MSE	CG-SE-CE	5.88	111.82	98.90
1	A	6	MSE	CG-SE-CE	-5.84	86.05	98.90
1	G	83	MSE	CG-SE-CE	5.75	111.54	98.90
1	H	6	MSE	CG-SE-CE	-5.66	86.44	98.90
1	H	83	MSE	CG-SE-CE	5.43	110.85	98.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	83	MSE	CG-SE-CE	5.40	110.79	98.90
1	D	6	MSE	CG-SE-CE	-5.30	87.23	98.90
1	G	415	MSE	CG-SE-CE	5.18	110.30	98.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	418	ASN	Peptide

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	3595	0	3436	12	1
1	B	3595	0	3430	6	0
1	C	3594	0	3412	21	0
1	D	3588	0	3414	16	0
1	E	3736	0	3548	34	0
1	F	3733	0	3541	12	0
1	G	3682	0	3498	14	0
1	H	3730	0	3545	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
4	A	441	0	0	5	1
4	B	395	0	0	1	0
4	C	431	0	0	6	0
4	D	389	0	0	0	0
4	E	455	0	0	5	0
4	F	426	0	0	1	0
4	G	456	0	0	3	0
4	H	420	0	0	0	0
All	All	32682	0	27824	127	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 2.

All (127) 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:C:279:TRP:CZ3	1:C:290:LYS:N	2.00	1.28
1:C:279:TRP:CH2	1:C:290:LYS:N	2.10	1.18
1:E:281:ARG:HD3	1:E:284:GLY:HA2	1.42	1.01
1:C:279:TRP:HZ3	1:C:290:LYS:N	1.67	0.89
1:C:417:ASP:OD2	1:C:419:LEU:HD22	1.78	0.83
1:C:6:MSE:SE	4:C:838:HOH:O	2.49	0.79
1:C:48:ARG:NE	1:C:50:GLU:OE1	2.20	0.74
1:E:282:VAL:HG11	1:E:415:MSE:SE	2.40	0.71
1:E:230:ARG:HH12	1:E:418:ASN:HD21	1.37	0.71
1:G:417:ASP:C	1:G:418:ASN:HD22	1.93	0.71
1:D:278:THR:OG1	1:D:279:TRP:N	2.18	0.71
1:E:233:ALA:HB1	1:E:236:THR:HB	1.73	0.70
1:C:279:TRP:HH2	1:C:290:LYS:N	1.86	0.69
1:H:282:VAL:CG1	1:H:415:MSE:CG	2.72	0.68
1:C:120:LYS:NZ	4:C:603:HOH:O	2.27	0.67
1:E:283:THR:CG2	1:E:415:MSE:HG3	2.24	0.67
1:E:301:ASN:O	1:E:304:THR:HG22	1.96	0.66
1:A:229:THR:HG22	4:A:606:HOH:O	1.94	0.66
1:D:278:THR:HG21	1:D:291:GLU:HB3	1.78	0.66
1:D:127:ARG:NH1	1:F:433:ARG:HD2	2.12	0.64
1:D:278:THR:HB	1:D:292:THR:H	1.62	0.64
4:A:762:HOH:O	1:D:152:SER:HB2	1.97	0.64
1:E:282:VAL:CG1	1:E:415:MSE:SE	2.96	0.64
1:G:417:ASP:O	1:G:418:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:THR:HG22	1:E:237:ASP:N	2.13	0.63
1:E:182:LYS:HE2	4:E:608:HOH:O	2.00	0.62
1:A:325:ASN:HB2	4:A:809:HOH:O	1.99	0.61
1:C:206:GLN:HG3	4:C:630:HOH:O	2.01	0.60
1:E:233:ALA:O	1:E:235:GLU:N	2.35	0.60
1:E:283:THR:CG2	1:E:415:MSE:CG	2.81	0.58
1:A:167:GLN:HG3	1:A:174:TRP:CE2	2.39	0.57
1:E:283:THR:HG23	1:E:415:MSE:HG3	1.87	0.57
1:G:182:LYS:HE2	4:G:926:HOH:O	2.03	0.57
1:F:409:ARG:HD3	1:F:414:LEU:HD21	1.87	0.57
1:G:301:ASN:O	1:G:304:THR:HG22	2.05	0.57
1:H:282:VAL:CG1	1:H:415:MSE:HG3	2.36	0.56
1:E:146:LYS:HE3	4:E:690:HOH:O	2.05	0.56
1:E:81:HIS:CD2	1:E:457:VAL:CG2	2.90	0.55
1:E:236:THR:CG2	1:E:237:ASP:N	2.69	0.55
1:C:381:ASN:HD22	1:C:384:ASN:H	1.54	0.54
1:F:456:VAL:HG12	1:F:457:VAL:HG23	1.90	0.54
1:D:278:THR:O	1:D:279:TRP:HB3	2.07	0.53
1:E:81:HIS:CD2	1:E:457:VAL:HG21	2.43	0.53
1:D:278:THR:O	1:D:279:TRP:CB	2.57	0.53
1:F:282:VAL:HG23	1:F:413:THR:HB	1.91	0.53
1:A:431[B]:ARG:CZ	4:A:727:HOH:O	2.57	0.53
1:D:278:THR:N	1:D:292:THR:O	2.38	0.53
1:B:457:VAL:HB	4:B:601:HOH:O	2.10	0.52
1:G:419:LEU:HD12	1:G:419:LEU:O	2.10	0.52
1:F:446:GLU:HB2	1:F:449:PHE:CD2	2.46	0.51
1:E:48:ARG:NE	1:E:50:GLU:OE1	2.43	0.51
1:F:146:LYS:HE3	4:F:702:HOH:O	2.11	0.51
1:H:282:VAL:HG12	1:H:415:MSE:CG	2.40	0.51
1:F:127:ARG:H	1:F:127:ARG:CZ	2.23	0.51
1:F:301:ASN:O	1:F:304:THR:HG22	2.11	0.51
1:B:143:GLY:HA3	1:B:159:PHE:CG	2.45	0.50
1:C:236:THR:OG1	1:C:237:ASP:N	2.45	0.50
1:G:297:LEU:HD22	1:G:304:THR:HG23	1.93	0.50
1:E:297:LEU:HD22	1:E:304:THR:HG23	1.94	0.50
1:H:143:GLY:HA3	1:H:159:PHE:CG	2.47	0.50
1:E:283:THR:HG21	1:E:415:MSE:HG3	1.92	0.49
1:H:282:VAL:CG1	1:H:415:MSE:HG2	2.40	0.49
1:E:234:HIS:NE2	1:E:283:THR:HB	2.27	0.49
1:F:143:GLY:HA3	1:F:159:PHE:CG	2.47	0.49
1:G:146:LYS:HE3	4:G:690:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:GLU:HG2	1:D:412:TYR:CZ	2.47	0.49
1:A:3:VAL:HG21	1:A:134:GLU:CG	2.43	0.49
1:E:381:ASN:ND2	4:E:603:HOH:O	2.46	0.48
1:E:407[B]:LYS:HA	4:E:748:HOH:O	2.13	0.48
1:D:143:GLY:HA3	1:D:159:PHE:CG	2.48	0.48
1:D:107:ASP:OD1	1:D:431:ARG:NH2	2.46	0.48
1:G:143:GLY:HA3	1:G:159:PHE:CG	2.48	0.48
1:H:302:LYS:NZ	1:H:393:PHE:O	2.43	0.48
1:C:381:ASN:HD21	1:C:383:ARG:HB2	1.78	0.48
1:B:48:ARG:NE	1:B:50:GLU:OE1	2.47	0.47
1:D:278:THR:CG2	1:D:291:GLU:HB3	2.45	0.47
1:H:285:ASP:HB3	1:H:288:ALA:HB3	1.96	0.47
1:E:407[A]:LYS:HA	4:E:748:HOH:O	2.15	0.47
1:E:82:GLU:O	1:E:458:SER:HB2	2.16	0.46
1:A:107:ASP:OD2	1:A:431[A]:ARG:NH1	2.45	0.46
1:C:206:GLN:HG3	4:C:983:HOH:O	2.16	0.46
1:B:301:ASN:O	1:B:304:THR:HG22	2.16	0.46
1:C:143:GLY:HA3	1:C:159:PHE:CG	2.51	0.45
1:A:143:GLY:HA3	1:A:159:PHE:CG	2.51	0.45
1:H:282:VAL:HG12	1:H:415:MSE:HG2	1.99	0.45
1:A:456:VAL:O	1:A:457:VAL:HB	2.16	0.45
1:G:297:LEU:HD22	1:G:304:THR:CG2	2.46	0.45
1:C:296:GLU:HG2	1:C:412:TYR:HE2	1.81	0.45
1:D:278:THR:CB	1:D:291:GLU:HB3	2.48	0.44
1:D:322:PHE:CE1	1:D:327:ARG:HD2	2.52	0.44
1:F:320:ILE:HG22	1:F:386:LYS:HE3	1.98	0.44
1:G:381:ASN:ND2	4:G:614:HOH:O	2.50	0.44
1:G:418:ASN:HB3	1:G:419:LEU:H	1.58	0.44
1:H:282:VAL:HG11	1:H:415:MSE:CG	2.48	0.44
1:H:298:LEU:O	1:H:302:LYS:HE2	2.17	0.44
1:A:167:GLN:HG3	1:A:174:TRP:CD2	2.52	0.44
1:A:3:VAL:CG2	1:A:134:GLU:HG2	2.47	0.44
1:G:303:HIS:HE1	1:G:307:ASP:O	2.01	0.44
1:H:282:VAL:HG11	1:H:415:MSE:HG3	1.99	0.44
1:C:348[A]:ASN:OD1	1:C:351:ARG:NH1	2.51	0.43
1:B:107:ASP:OD2	1:B:431:ARG:NH1	2.51	0.43
1:B:107:ASP:OD1	1:B:431:ARG:NH2	2.52	0.43
1:C:124:ASN:HB3	1:F:235:GLU:O	2.19	0.43
1:C:279:TRP:HA	1:C:291:GLU:HB3	2.01	0.43
1:E:383:ARG:HA	1:E:383:ARG:HD2	1.90	0.43
1:D:296:GLU:CG	1:D:412:TYR:CZ	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:PHE:HA	1:E:438:GLU:O	2.20	0.42
1:A:268:ARG:NH2	4:A:603:HOH:O	2.49	0.42
1:E:143:GLY:HA3	1:E:159:PHE:CG	2.54	0.42
1:H:302:LYS:HE3	1:H:396:ASP:HB3	2.02	0.42
1:E:372:ASN:HB2	1:E:379:ILE:HD11	2.00	0.42
1:E:297:LEU:HD22	1:E:304:THR:CG2	2.49	0.42
1:G:232:LYS:NZ	1:G:418:ASN:HD21	2.18	0.42
1:C:212:LYS:NZ	4:C:619:HOH:O	2.52	0.41
1:C:217:SER:O	1:C:259:GLN:HA	2.20	0.41
1:F:446:GLU:HB2	1:F:449:PHE:HD2	1.84	0.41
1:D:372:ASN:HB2	1:D:379:ILE:HD11	2.02	0.41
1:E:236:THR:CG2	1:E:237:ASP:H	2.31	0.41
1:E:81:HIS:CG	1:E:457:VAL:CG2	3.04	0.41
1:A:3:VAL:HG21	1:A:134:GLU:HG3	2.03	0.41
1:G:302:LYS:HD2	1:G:313:ASP:OD1	2.21	0.41
1:E:419:LEU:O	1:E:419:LEU:HD12	2.20	0.41
1:H:296:GLU:HG2	1:H:412:TYR:CE2	2.56	0.41
1:C:381:ASN:HB2	4:C:777:HOH:O	2.20	0.40
1:H:298:LEU:O	1:H:302:LYS:CE	2.69	0.40
1:E:283:THR:HG23	1:E:415:MSE:CG	2.50	0.40
1:E:282:VAL:HG12	1:E:283:THR:HG23	2.03	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)
1:A:340:TYR:OH	1:A:431[B]:ARG:NH1[1_655]	1.86	0.34
4:A:687:HOH:O	4:A:975:HOH:O[1_455]	2.11	0.09

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	438/498 (88%)	422 (96%)	15 (3%)	1 (0%)	47 26
1	B	438/498 (88%)	425 (97%)	13 (3%)	0	100 100
1	C	436/498 (88%)	419 (96%)	11 (2%)	6 (1%)	11 2
1	D	435/498 (87%)	425 (98%)	10 (2%)	0	100 100
1	E	461/498 (93%)	439 (95%)	15 (3%)	7 (2%)	10 2
1	F	461/498 (93%)	450 (98%)	9 (2%)	2 (0%)	34 15
1	G	452/498 (91%)	438 (97%)	12 (3%)	2 (0%)	34 15
1	H	460/498 (92%)	454 (99%)	6 (1%)	0	100 100
All	All	3581/3984 (90%)	3472 (97%)	91 (2%)	18 (0%)	29 11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	44	ASP
1	E	148	ALA
1	E	237	ASP
1	E	238	ASP
1	E	286	ASN
1	E	417	ASP
1	C	417	ASP
1	C	419	LEU
1	G	417	ASP
1	E	234	HIS
1	F	286	ASN
1	G	286	ASN
1	A	234	HIS
1	C	291	GLU
1	C	43	ALA
1	F	284	GLY
1	E	416	PRO
1	C	84	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	401/434 (92%)	398 (99%)	3 (1%)	84 73
1	B	401/434 (92%)	396 (99%)	5 (1%)	71 54
1	C	401/434 (92%)	396 (99%)	5 (1%)	71 54
1	D	402/434 (93%)	400 (100%)	2 (0%)	88 80
1	E	417/434 (96%)	414 (99%)	3 (1%)	84 73
1	F	417/434 (96%)	412 (99%)	5 (1%)	71 54
1	G	410/434 (94%)	407 (99%)	3 (1%)	84 73
1	H	416/434 (96%)	411 (99%)	5 (1%)	71 54
All	All	3265/3472 (94%)	3234 (99%)	31 (1%)	76 65

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	SER
1	A	278	THR
1	A	333	THR
1	B	42	ASP
1	B	151	SER
1	B	304	THR
1	B	333	THR
1	B	374	GLU
1	C	83	MSE
1	C	236	THR
1	C	238	ASP
1	C	290	LYS
1	C	412	TYR
1	D	333	THR
1	D	348	ASN
1	E	151	SER
1	E	285	ASP
1	E	419	LEU
1	F	127	ARG
1	F	151	SER
1	F	282	VAL
1	F	304	THR
1	F	333	THR
1	G	303	HIS
1	G	304	THR
1	G	419	LEU
1	H	127	ARG

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Mol	Chain	Res	Type
1	H	151	SER
1	H	200	CYS
1	H	333	THR
1	H	448	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	206	GLN
1	C	381	ASN
1	E	140	ASN
1	F	286	ASN
1	G	381	ASN
1	H	206	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	435/498 (87%)	-0.54	10 (2%)	60	59	16, 24, 56, 102	0
1	B	435/498 (87%)	-0.50	8 (1%)	68	67	16, 27, 68, 98	0
1	C	434/498 (87%)	-0.49	13 (2%)	50	48	15, 24, 56, 114	0
1	D	432/498 (86%)	-0.50	9 (2%)	63	62	16, 27, 63, 116	0
1	E	450/498 (90%)	-0.44	14 (3%)	49	46	15, 24, 56, 111	0
1	F	451/498 (90%)	-0.52	2 (0%)	92	92	14, 26, 61, 99	0
1	G	444/498 (89%)	-0.47	8 (1%)	68	67	14, 23, 53, 98	0
1	H	451/498 (90%)	-0.55	5 (1%)	80	80	15, 27, 59, 87	0
All	All	3532/3984 (88%)	-0.50	69 (1%)	65	64	14, 25, 61, 116	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	279	TRP	10.6
1	C	236	THR	10.1
1	C	280	GLY	8.3
1	F	284	GLY	8.0
1	G	285	ASP	6.6
1	B	290	LYS	5.6
1	C	418	ASN	5.4
1	A	235	GLU	5.1
1	C	279	TRP	5.0
1	B	414	LEU	4.8
1	E	235	GLU	4.8
1	A	237	ASP	4.7
1	H	418	ASN	4.6
1	C	412	TYR	4.6
1	C	411	TYR	4.5
1	G	43	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	417	ASP	3.9
1	C	44	ASP	3.8
1	E	285	ASP	3.8
1	A	411	TYR	3.8
1	G	417	ASP	3.7
1	H	43	ALA	3.5
1	H	284	GLY	3.3
1	A	45	GLY	3.3
1	G	284	GLY	3.3
1	E	419	LEU	3.2
1	D	413	THR	3.2
1	E	284	GLY	3.2
1	C	290	LYS	3.1
1	C	45	GLY	3.1
1	E	238	ASP	3.0
1	A	43	ALA	3.0
1	D	412	TYR	2.9
1	B	411	TYR	2.9
1	D	237	ASP	2.8
1	G	286	ASN	2.8
1	G	419	LEU	2.8
1	E	237	ASP	2.8
1	A	234	HIS	2.7
1	B	44	ASP	2.7
1	A	238	ASP	2.7
1	B	279	TRP	2.6
1	E	234	HIS	2.6
1	C	238	ASP	2.6
1	G	42	ASP	2.6
1	F	286	ASN	2.6
1	E	42	ASP	2.5
1	C	42	ASP	2.5
1	E	416	PRO	2.4
1	D	291	GLU	2.4
1	C	237	ASP	2.4
1	A	290	LYS	2.3
1	B	233	ALA	2.3
1	E	282	VAL	2.3
1	B	291	GLU	2.3
1	E	43	ALA	2.3
1	H	286	ASN	2.3
1	D	45	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	236	THR	2.3
1	A	410	SER	2.2
1	E	44	ASP	2.2
1	B	449	PHE	2.2
1	D	309	ILE	2.2
1	C	278	THR	2.1
1	G	416	PRO	2.1
1	H	288	ALA	2.1
1	D	414	LEU	2.1
1	E	233	ALA	2.0
1	D	278	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	F	502	1/1	0.98	0.03	52,52,52,52	0
3	CA	H	502	1/1	0.98	0.03	48,48,48,48	0
3	CA	D	502	1/1	0.99	0.03	55,55,55,55	0
3	CA	B	502	1/1	0.99	0.03	51,51,51,51	0
3	CA	E	502	1/1	0.99	0.05	46,46,46,46	0
3	CA	C	502	1/1	1.00	0.06	50,50,50,50	0
2	ZN	H	501	1/1	1.00	0.05	29,29,29,29	0
2	ZN	D	501	1/1	1.00	0.05	26,26,26,26	0
2	ZN	C	501	1/1	1.00	0.05	24,24,24,24	0
3	CA	A	502	1/1	1.00	0.04	47,47,47,47	0
2	ZN	F	501	1/1	1.00	0.04	29,29,29,29	0
2	ZN	E	501	1/1	1.00	0.06	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	501	1/1	1.00	0.04	26,26,26,26	0
2	ZN	A	501	1/1	1.00	0.05	23,23,23,23	0
3	CA	G	502	1/1	1.00	0.03	43,43,43,43	0
2	ZN	G	501	1/1	1.00	0.06	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.