Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2025 – 06:11 pm GMT

PDB ID	:	9H68
Title	:	Crystal Structure of the spore gernation lytic transglycosylase SleC from Clostridioides difficile in its zymogenic form (prepro-SleC)
Authors	:	Molina, R.; Garay-Alvarez, A.; Hermoso, J.A.
Deposited on	:	2024-10-23
Resolution	:	2.10 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:

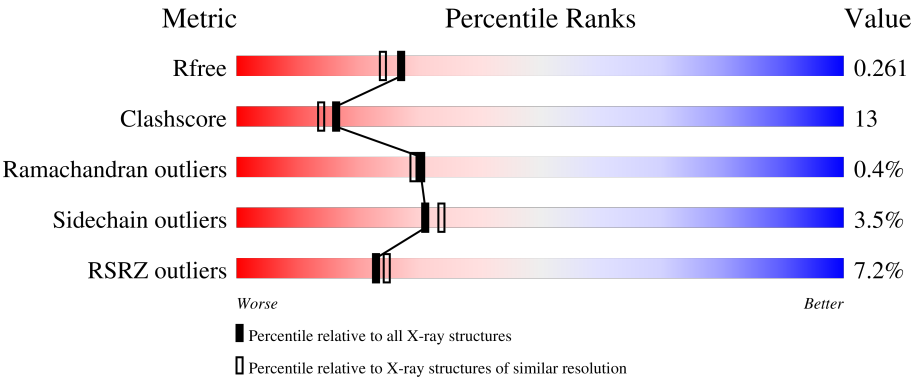
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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 <=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	480	4% 64% 21% • 14%
1	B	480	3% 63% 22% 15%
1	C	480	10% 65% 18% • 15%
1	D	480	8% 60% 23% • 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13534 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 Spore cortex-lytic enzyme pre-pro-form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3274	2102	533	633	6			
1	D	404	Total	C	N	O	S	0	0	0
			3199	2052	520	621	6			
1	B	410	Total	C	N	O	S	0	0	0
			3256	2090	530	630	6			
1	C	406	Total	C	N	O	S	0	0	0
			3216	2061	525	624	6			

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-56	MET	-	initiating methionine	UNP Q188Z5
A	-55	GLY	-	expression tag	UNP Q188Z5
A	-54	SER	-	expression tag	UNP Q188Z5
A	-53	SER	-	expression tag	UNP Q188Z5
A	-52	HIS	-	expression tag	UNP Q188Z5
A	-51	HIS	-	expression tag	UNP Q188Z5
A	-50	HIS	-	expression tag	UNP Q188Z5
A	-49	HIS	-	expression tag	UNP Q188Z5
A	-48	HIS	-	expression tag	UNP Q188Z5
A	-47	HIS	-	expression tag	UNP Q188Z5
A	-46	SER	-	expression tag	UNP Q188Z5
A	-45	SER	-	expression tag	UNP Q188Z5
A	-44	GLY	-	expression tag	UNP Q188Z5
A	-43	SER	-	expression tag	UNP Q188Z5
A	-42	ALA	-	expression tag	UNP Q188Z5
A	-41	TRP	-	expression tag	UNP Q188Z5
A	-40	SER	-	expression tag	UNP Q188Z5
A	-39	HIS	-	expression tag	UNP Q188Z5
A	-38	PRO	-	expression tag	UNP Q188Z5
A	-37	GLN	-	expression tag	UNP Q188Z5
A	-36	PHE	-	expression tag	UNP Q188Z5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	GLU	-	expression tag	UNP Q188Z5
A	-34	LYS	-	expression tag	UNP Q188Z5
A	-33	GLY	-	expression tag	UNP Q188Z5
A	-32	GLY	-	expression tag	UNP Q188Z5
A	-31	GLY	-	expression tag	UNP Q188Z5
A	-30	SER	-	expression tag	UNP Q188Z5
A	-29	GLY	-	expression tag	UNP Q188Z5
A	-28	GLY	-	expression tag	UNP Q188Z5
A	-27	GLY	-	expression tag	UNP Q188Z5
A	-26	SER	-	expression tag	UNP Q188Z5
A	-25	GLY	-	expression tag	UNP Q188Z5
A	-24	GLY	-	expression tag	UNP Q188Z5
A	-23	SER	-	expression tag	UNP Q188Z5
A	-22	ALA	-	expression tag	UNP Q188Z5
A	-21	TRP	-	expression tag	UNP Q188Z5
A	-20	SER	-	expression tag	UNP Q188Z5
A	-19	HIS	-	expression tag	UNP Q188Z5
A	-18	PRO	-	expression tag	UNP Q188Z5
A	-17	GLN	-	expression tag	UNP Q188Z5
A	-16	PHE	-	expression tag	UNP Q188Z5
A	-15	GLU	-	expression tag	UNP Q188Z5
A	-14	LYS	-	expression tag	UNP Q188Z5
A	-13	SER	-	expression tag	UNP Q188Z5
A	-12	ASN	-	expression tag	UNP Q188Z5
A	-11	ASN	-	expression tag	UNP Q188Z5
A	-10	ASN	-	expression tag	UNP Q188Z5
A	-9	LEU	-	expression tag	UNP Q188Z5
A	-8	GLY	-	expression tag	UNP Q188Z5
A	-7	GLU	-	expression tag	UNP Q188Z5
A	-6	ASN	-	expression tag	UNP Q188Z5
A	-5	LEU	-	expression tag	UNP Q188Z5
A	-4	TYR	-	expression tag	UNP Q188Z5
A	-3	PHE	-	expression tag	UNP Q188Z5
A	-2	GLN	-	expression tag	UNP Q188Z5
A	-1	GLY	-	expression tag	UNP Q188Z5
A	0	HIS	-	expression tag	UNP Q188Z5
D	-56	MET	-	initiating methionine	UNP Q188Z5
D	-55	GLY	-	expression tag	UNP Q188Z5
D	-54	SER	-	expression tag	UNP Q188Z5
D	-53	SER	-	expression tag	UNP Q188Z5
D	-52	HIS	-	expression tag	UNP Q188Z5
D	-51	HIS	-	expression tag	UNP Q188Z5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-50	HIS	-	expression tag	UNP Q188Z5
D	-49	HIS	-	expression tag	UNP Q188Z5
D	-48	HIS	-	expression tag	UNP Q188Z5
D	-47	HIS	-	expression tag	UNP Q188Z5
D	-46	SER	-	expression tag	UNP Q188Z5
D	-45	SER	-	expression tag	UNP Q188Z5
D	-44	GLY	-	expression tag	UNP Q188Z5
D	-43	SER	-	expression tag	UNP Q188Z5
D	-42	ALA	-	expression tag	UNP Q188Z5
D	-41	TRP	-	expression tag	UNP Q188Z5
D	-40	SER	-	expression tag	UNP Q188Z5
D	-39	HIS	-	expression tag	UNP Q188Z5
D	-38	PRO	-	expression tag	UNP Q188Z5
D	-37	GLN	-	expression tag	UNP Q188Z5
D	-36	PHE	-	expression tag	UNP Q188Z5
D	-35	GLU	-	expression tag	UNP Q188Z5
D	-34	LYS	-	expression tag	UNP Q188Z5
D	-33	GLY	-	expression tag	UNP Q188Z5
D	-32	GLY	-	expression tag	UNP Q188Z5
D	-31	GLY	-	expression tag	UNP Q188Z5
D	-30	SER	-	expression tag	UNP Q188Z5
D	-29	GLY	-	expression tag	UNP Q188Z5
D	-28	GLY	-	expression tag	UNP Q188Z5
D	-27	GLY	-	expression tag	UNP Q188Z5
D	-26	SER	-	expression tag	UNP Q188Z5
D	-25	GLY	-	expression tag	UNP Q188Z5
D	-24	GLY	-	expression tag	UNP Q188Z5
D	-23	SER	-	expression tag	UNP Q188Z5
D	-22	ALA	-	expression tag	UNP Q188Z5
D	-21	TRP	-	expression tag	UNP Q188Z5
D	-20	SER	-	expression tag	UNP Q188Z5
D	-19	HIS	-	expression tag	UNP Q188Z5
D	-18	PRO	-	expression tag	UNP Q188Z5
D	-17	GLN	-	expression tag	UNP Q188Z5
D	-16	PHE	-	expression tag	UNP Q188Z5
D	-15	GLU	-	expression tag	UNP Q188Z5
D	-14	LYS	-	expression tag	UNP Q188Z5
D	-13	SER	-	expression tag	UNP Q188Z5
D	-12	ASN	-	expression tag	UNP Q188Z5
D	-11	ASN	-	expression tag	UNP Q188Z5
D	-10	ASN	-	expression tag	UNP Q188Z5
D	-9	LEU	-	expression tag	UNP Q188Z5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	GLY	-	expression tag	UNP Q188Z5
D	-7	GLU	-	expression tag	UNP Q188Z5
D	-6	ASN	-	expression tag	UNP Q188Z5
D	-5	LEU	-	expression tag	UNP Q188Z5
D	-4	TYR	-	expression tag	UNP Q188Z5
D	-3	PHE	-	expression tag	UNP Q188Z5
D	-2	GLN	-	expression tag	UNP Q188Z5
D	-1	GLY	-	expression tag	UNP Q188Z5
D	0	HIS	-	expression tag	UNP Q188Z5
B	-56	MET	-	initiating methionine	UNP Q188Z5
B	-55	GLY	-	expression tag	UNP Q188Z5
B	-54	SER	-	expression tag	UNP Q188Z5
B	-53	SER	-	expression tag	UNP Q188Z5
B	-52	HIS	-	expression tag	UNP Q188Z5
B	-51	HIS	-	expression tag	UNP Q188Z5
B	-50	HIS	-	expression tag	UNP Q188Z5
B	-49	HIS	-	expression tag	UNP Q188Z5
B	-48	HIS	-	expression tag	UNP Q188Z5
B	-47	HIS	-	expression tag	UNP Q188Z5
B	-46	SER	-	expression tag	UNP Q188Z5
B	-45	SER	-	expression tag	UNP Q188Z5
B	-44	GLY	-	expression tag	UNP Q188Z5
B	-43	SER	-	expression tag	UNP Q188Z5
B	-42	ALA	-	expression tag	UNP Q188Z5
B	-41	TRP	-	expression tag	UNP Q188Z5
B	-40	SER	-	expression tag	UNP Q188Z5
B	-39	HIS	-	expression tag	UNP Q188Z5
B	-38	PRO	-	expression tag	UNP Q188Z5
B	-37	GLN	-	expression tag	UNP Q188Z5
B	-36	PHE	-	expression tag	UNP Q188Z5
B	-35	GLU	-	expression tag	UNP Q188Z5
B	-34	LYS	-	expression tag	UNP Q188Z5
B	-33	GLY	-	expression tag	UNP Q188Z5
B	-32	GLY	-	expression tag	UNP Q188Z5
B	-31	GLY	-	expression tag	UNP Q188Z5
B	-30	SER	-	expression tag	UNP Q188Z5
B	-29	GLY	-	expression tag	UNP Q188Z5
B	-28	GLY	-	expression tag	UNP Q188Z5
B	-27	GLY	-	expression tag	UNP Q188Z5
B	-26	SER	-	expression tag	UNP Q188Z5
B	-25	GLY	-	expression tag	UNP Q188Z5
B	-24	GLY	-	expression tag	UNP Q188Z5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	SER	-	expression tag	UNP Q188Z5
B	-22	ALA	-	expression tag	UNP Q188Z5
B	-21	TRP	-	expression tag	UNP Q188Z5
B	-20	SER	-	expression tag	UNP Q188Z5
B	-19	HIS	-	expression tag	UNP Q188Z5
B	-18	PRO	-	expression tag	UNP Q188Z5
B	-17	GLN	-	expression tag	UNP Q188Z5
B	-16	PHE	-	expression tag	UNP Q188Z5
B	-15	GLU	-	expression tag	UNP Q188Z5
B	-14	LYS	-	expression tag	UNP Q188Z5
B	-13	SER	-	expression tag	UNP Q188Z5
B	-12	ASN	-	expression tag	UNP Q188Z5
B	-11	ASN	-	expression tag	UNP Q188Z5
B	-10	ASN	-	expression tag	UNP Q188Z5
B	-9	LEU	-	expression tag	UNP Q188Z5
B	-8	GLY	-	expression tag	UNP Q188Z5
B	-7	GLU	-	expression tag	UNP Q188Z5
B	-6	ASN	-	expression tag	UNP Q188Z5
B	-5	LEU	-	expression tag	UNP Q188Z5
B	-4	TYR	-	expression tag	UNP Q188Z5
B	-3	PHE	-	expression tag	UNP Q188Z5
B	-2	GLN	-	expression tag	UNP Q188Z5
B	-1	GLY	-	expression tag	UNP Q188Z5
B	0	HIS	-	expression tag	UNP Q188Z5
C	-56	MET	-	initiating methionine	UNP Q188Z5
C	-55	GLY	-	expression tag	UNP Q188Z5
C	-54	SER	-	expression tag	UNP Q188Z5
C	-53	SER	-	expression tag	UNP Q188Z5
C	-52	HIS	-	expression tag	UNP Q188Z5
C	-51	HIS	-	expression tag	UNP Q188Z5
C	-50	HIS	-	expression tag	UNP Q188Z5
C	-49	HIS	-	expression tag	UNP Q188Z5
C	-48	HIS	-	expression tag	UNP Q188Z5
C	-47	HIS	-	expression tag	UNP Q188Z5
C	-46	SER	-	expression tag	UNP Q188Z5
C	-45	SER	-	expression tag	UNP Q188Z5
C	-44	GLY	-	expression tag	UNP Q188Z5
C	-43	SER	-	expression tag	UNP Q188Z5
C	-42	ALA	-	expression tag	UNP Q188Z5
C	-41	TRP	-	expression tag	UNP Q188Z5
C	-40	SER	-	expression tag	UNP Q188Z5
C	-39	HIS	-	expression tag	UNP Q188Z5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-38	PRO	-	expression tag	UNP Q188Z5
C	-37	GLN	-	expression tag	UNP Q188Z5
C	-36	PHE	-	expression tag	UNP Q188Z5
C	-35	GLU	-	expression tag	UNP Q188Z5
C	-34	LYS	-	expression tag	UNP Q188Z5
C	-33	GLY	-	expression tag	UNP Q188Z5
C	-32	GLY	-	expression tag	UNP Q188Z5
C	-31	GLY	-	expression tag	UNP Q188Z5
C	-30	SER	-	expression tag	UNP Q188Z5
C	-29	GLY	-	expression tag	UNP Q188Z5
C	-28	GLY	-	expression tag	UNP Q188Z5
C	-27	GLY	-	expression tag	UNP Q188Z5
C	-26	SER	-	expression tag	UNP Q188Z5
C	-25	GLY	-	expression tag	UNP Q188Z5
C	-24	GLY	-	expression tag	UNP Q188Z5
C	-23	SER	-	expression tag	UNP Q188Z5
C	-22	ALA	-	expression tag	UNP Q188Z5
C	-21	TRP	-	expression tag	UNP Q188Z5
C	-20	SER	-	expression tag	UNP Q188Z5
C	-19	HIS	-	expression tag	UNP Q188Z5
C	-18	PRO	-	expression tag	UNP Q188Z5
C	-17	GLN	-	expression tag	UNP Q188Z5
C	-16	PHE	-	expression tag	UNP Q188Z5
C	-15	GLU	-	expression tag	UNP Q188Z5
C	-14	LYS	-	expression tag	UNP Q188Z5
C	-13	SER	-	expression tag	UNP Q188Z5
C	-12	ASN	-	expression tag	UNP Q188Z5
C	-11	ASN	-	expression tag	UNP Q188Z5
C	-10	ASN	-	expression tag	UNP Q188Z5
C	-9	LEU	-	expression tag	UNP Q188Z5
C	-8	GLY	-	expression tag	UNP Q188Z5
C	-7	GLU	-	expression tag	UNP Q188Z5
C	-6	ASN	-	expression tag	UNP Q188Z5
C	-5	LEU	-	expression tag	UNP Q188Z5
C	-4	TYR	-	expression tag	UNP Q188Z5
C	-3	PHE	-	expression tag	UNP Q188Z5
C	-2	GLN	-	expression tag	UNP Q188Z5
C	-1	GLY	-	expression tag	UNP Q188Z5
C	0	HIS	-	expression tag	UNP Q188Z5

- Molecule 2 is water.

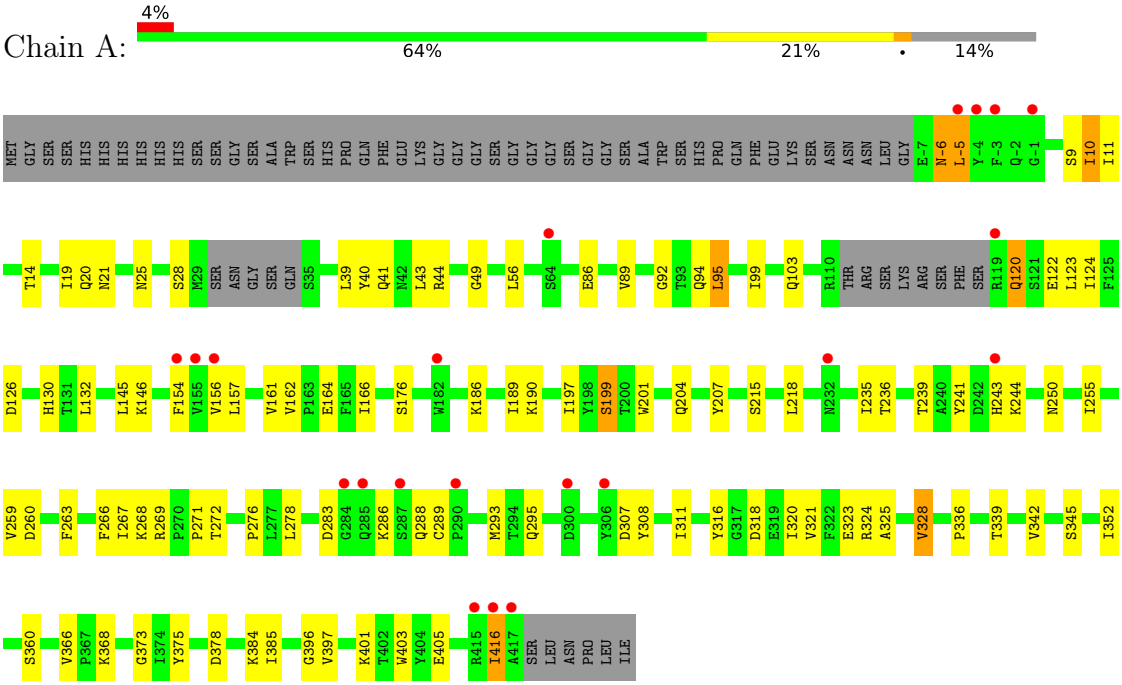
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	130	Total O 130 130	0	0
2	D	143	Total O 143 143	0	0
2	B	168	Total O 168 168	0	0
2	C	148	Total O 148 148	0	0

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.

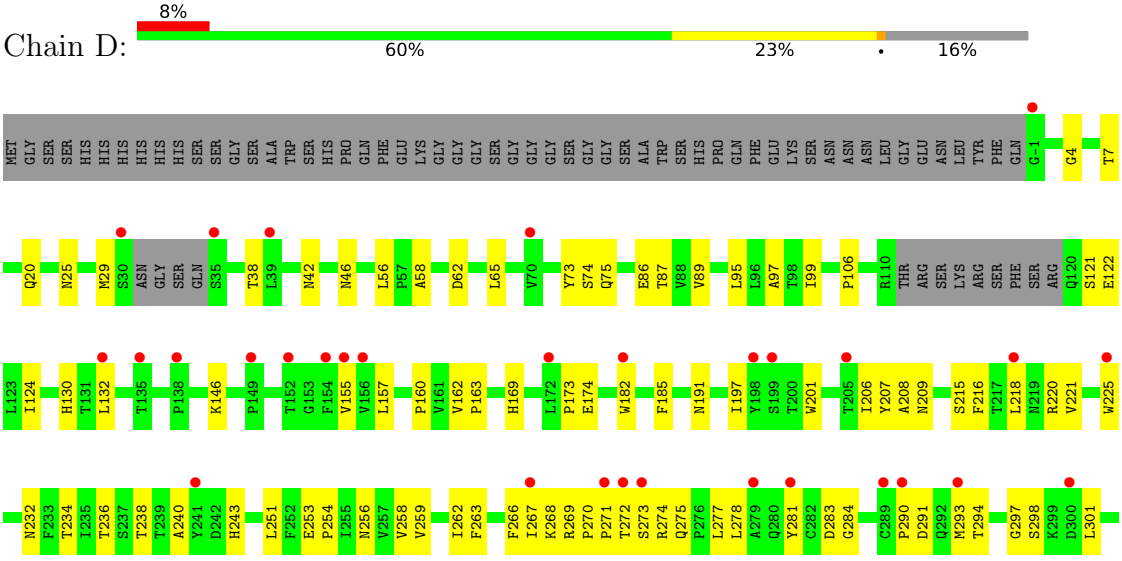
• Molecule 1: Spore cortex-lytic enzyme pre-pro-form

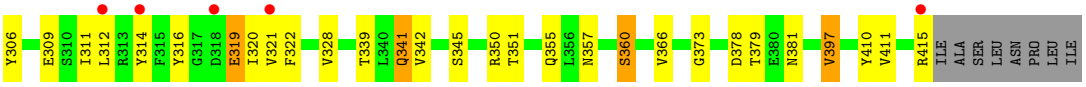
Chain A:



• Molecule 1: Spore cortex-lytic enzyme pre-pro-form

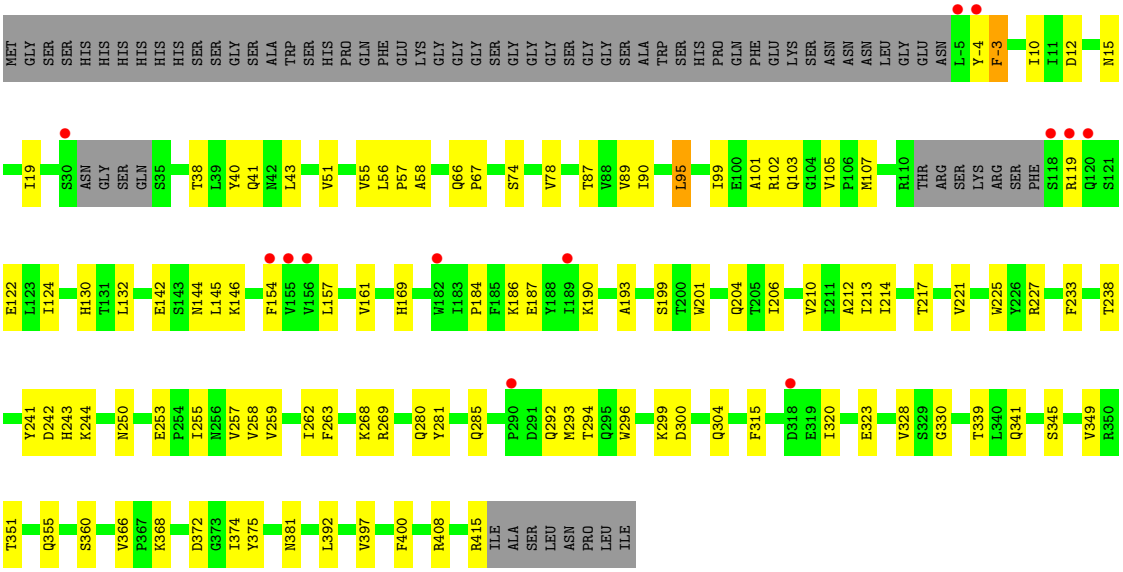
Chain D:





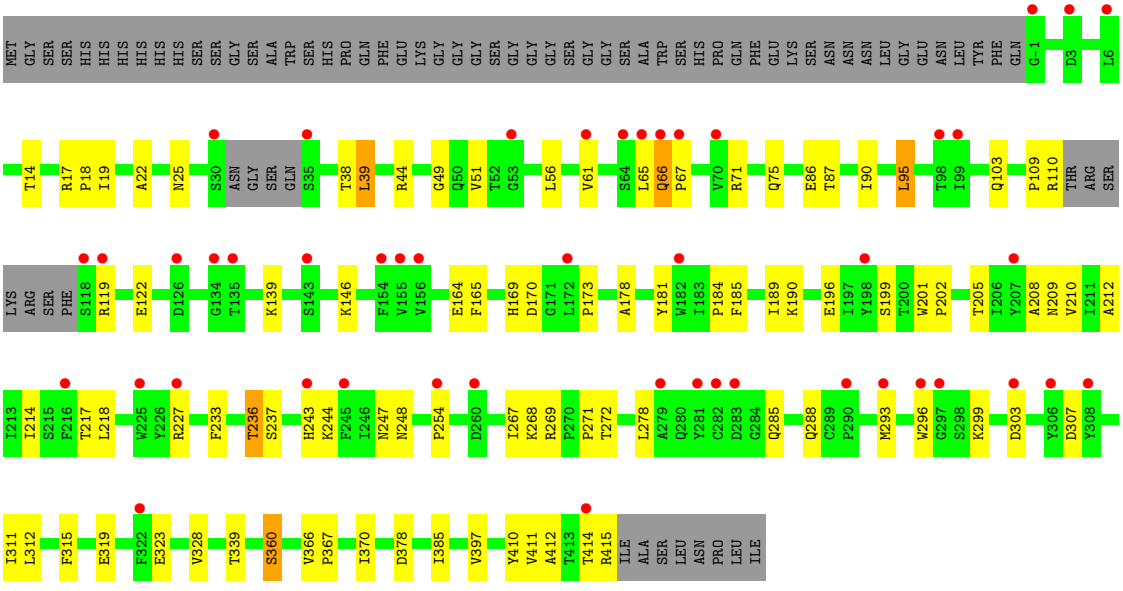
• Molecule 1: Spore cortex-lytic enzyme pre-pro-form

Chain B:



• Molecule 1: Spore cortex-lytic enzyme pre-pro-form

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.43Å 89.78Å 99.62Å 76.90° 75.87° 89.12°	Depositor
Resolution (Å)	72.90 – 2.10 72.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	57.3 (72.90-2.10) 57.3 (72.90-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.211 , 0.261 0.211 , 0.261	Depositor DCC
R_{free} test set	6380 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13534	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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

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	0.47	0/3361	0.66	1/4595 (0.0%)
1	B	0.48	0/3343	0.65	0/4570
1	C	0.42	1/3301 (0.0%)	0.60	0/4513
1	D	0.46	0/3284	0.63	0/4491
All	All	0.46	1/13289 (0.0%)	0.64	1/18169 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	GLN	CD-OE1	-5.49	1.11	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	-5	LEU	CA-CB-CG	5.78	128.59	115.30

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	A	3274	0	3176	82	0
1	B	3256	0	3158	87	0
1	C	3216	0	3121	77	0
1	D	3199	0	3103	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	130	0	0	34	0
2	B	168	0	0	48	0
2	C	148	0	0	35	0
2	D	143	0	0	35	0
All	All	13534	0	12558	326	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 13.

All (326) 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:D:294:THR:HG22	1:D:297:GLY:H	1.25	1.02
1:A:259:VAL:HG11	2:A:502:HOH:O	1.66	0.94
1:D:267:ILE:HD11	1:D:312:LEU:HD13	1.56	0.87
1:A:268:LYS:HD3	1:A:323:GLU:HG3	1.55	0.86
1:A:146:LYS:HE2	1:A:278:LEU:HD22	1.56	0.86
1:B:130:HIS:HD2	1:B:132:LEU:H	1.22	0.84
1:B:268:LYS:HD3	1:B:323:GLU:HG3	1.62	0.81
1:D:351:THR:HB	2:D:502:HOH:O	1.83	0.78
1:A:336:PRO:HD3	2:A:598:HOH:O	1.83	0.77
1:D:75:GLN:HG2	2:D:548:HOH:O	1.85	0.77
1:D:218:LEU:HB2	2:D:573:HOH:O	1.85	0.76
1:B:328:VAL:HG23	2:B:514:HOH:O	1.86	0.76
1:D:163:PRO:HD2	2:D:635:HOH:O	1.87	0.74
1:D:266:PHE:HA	2:D:503:HOH:O	1.86	0.73
1:C:267:ILE:HD11	1:C:312:LEU:HD13	1.69	0.73
1:D:410:TYR:HB2	2:D:567:HOH:O	1.89	0.73
1:B:130:HIS:CD2	1:B:132:LEU:H	2.06	0.73
1:D:130:HIS:HD2	1:D:132:LEU:H	1.37	0.72
1:D:220:ARG:HG2	2:D:504:HOH:O	1.89	0.72
1:D:73:TYR:HD1	2:D:548:HOH:O	1.72	0.72
1:C:173:PRO:HG3	1:C:236:THR:HG21	1.72	0.72
1:C:109:PRO:HD3	2:C:505:HOH:O	1.91	0.70
1:C:87:THR:HB	1:C:122:GLU:HG2	1.76	0.68
1:D:355:GLN:HB3	2:D:567:HOH:O	1.94	0.68
1:B:58:ALA:HA	1:B:74:SER:OG	1.94	0.68
1:A:267:ILE:HA	2:A:538:HOH:O	1.94	0.67
1:B:12:ASP:HA	2:B:540:HOH:O	1.94	0.67
1:D:269:ARG:HG2	1:D:269:ARG:HH11	1.58	0.67
1:D:415:ARG:HB2	1:C:415:ARG:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ASN:HA	2:D:606:HOH:O	1.94	0.67
1:B:341:GLN:HB3	1:B:397:VAL:HG22	1.76	0.67
1:A:130:HIS:CD2	1:A:132:LEU:H	2.13	0.66
1:A:324:ARG:HD2	2:A:615:HOH:O	1.94	0.66
1:A:190:LYS:HG3	2:A:502:HOH:O	1.95	0.66
1:A:218:LEU:HB2	2:A:571:HOH:O	1.94	0.66
1:A:130:HIS:HD2	1:A:132:LEU:H	1.41	0.66
1:B:296:TRP:HA	2:B:641:HOH:O	1.95	0.65
1:A:215:SER:HA	2:A:571:HOH:O	1.96	0.65
1:B:57:PRO:HD2	2:B:565:HOH:O	1.97	0.65
1:C:146:LYS:HE2	1:C:278:LEU:HD22	1.77	0.65
1:A:235:ILE:HG22	2:A:501:HOH:O	1.98	0.64
1:B:293:MET:HG3	1:B:315:PHE:CD2	2.32	0.64
1:C:75:GLN:HG3	2:C:523:HOH:O	1.98	0.64
1:D:89:VAL:HB	1:D:124:ILE:HD13	1.80	0.64
1:B:58:ALA:HB3	2:B:506:HOH:O	1.98	0.63
1:C:367:PRO:HD2	2:C:538:HOH:O	1.97	0.62
1:C:25:ASN:HB3	2:C:511:HOH:O	1.98	0.62
1:B:345:SER:HA	2:B:512:HOH:O	1.98	0.62
1:D:381:ASN:HB2	2:D:609:HOH:O	1.98	0.62
1:D:215:SER:HA	2:D:573:HOH:O	1.98	0.62
1:C:67:PRO:HD3	1:C:296:TRP:CD2	2.35	0.61
1:A:204:GLN:HA	2:A:508:HOH:O	2.01	0.61
1:C:360:SER:HB2	1:C:366:VAL:O	2.00	0.61
1:A:295:GLN:HB3	2:A:507:HOH:O	2.00	0.61
1:D:415:ARG:HH11	1:C:415:ARG:HB3	1.66	0.60
1:B:269:ARG:HB2	1:B:320:ILE:HG22	1.84	0.60
1:C:185:PHE:HD2	2:C:542:HOH:O	1.85	0.60
1:C:212:ALA:HA	2:C:534:HOH:O	2.01	0.60
1:A:39:LEU:HB3	2:A:608:HOH:O	2.01	0.60
1:A:197:ILE:HG22	2:A:507:HOH:O	2.01	0.59
1:A:266:PHE:CD1	1:A:276:PRO:HB3	2.36	0.59
1:A:189:ILE:HG22	2:A:520:HOH:O	2.02	0.59
1:B:56:LEU:HB2	1:B:95:LEU:HD22	1.85	0.59
1:B:214:ILE:HD11	2:B:634:HOH:O	2.01	0.59
1:D:130:HIS:CD2	1:D:132:LEU:H	2.20	0.59
1:A:259:VAL:HG12	2:A:558:HOH:O	2.03	0.59
1:C:311:ILE:HG22	2:C:513:HOH:O	2.03	0.59
1:B:107:MET:HB2	2:B:540:HOH:O	2.03	0.58
1:B:258:VAL:HB	2:B:584:HOH:O	2.04	0.58
1:C:385:ILE:HB	2:C:538:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:TRP:HB3	2:C:605:HOH:O	2.03	0.58
1:B:244:LYS:HD3	2:B:501:HOH:O	2.04	0.58
1:C:14:THR:HG23	2:C:505:HOH:O	2.03	0.57
1:C:178:ALA:HB1	2:C:502:HOH:O	2.05	0.57
1:B:206:ILE:HD11	2:B:515:HOH:O	2.05	0.57
1:B:381:ASN:HB2	2:B:640:HOH:O	2.04	0.57
1:C:271:PRO:HG3	1:C:319:GLU:O	2.05	0.56
1:B:10:ILE:HD13	1:B:105:VAL:HB	1.87	0.56
1:C:119:ARG:H	1:C:119:ARG:HD2	1.70	0.56
1:D:301:LEU:HB3	1:D:306:TYR:HD2	1.68	0.56
1:D:360:SER:HB2	1:D:366:VAL:O	2.05	0.56
1:B:103:GLN:HG2	2:B:508:HOH:O	2.05	0.56
1:A:25:ASN:HB3	2:A:530:HOH:O	2.06	0.56
1:D:86:GLU:HG2	1:D:122:GLU:HA	1.87	0.56
1:D:97:ALA:HB1	2:D:534:HOH:O	2.06	0.55
1:D:379:THR:HB	2:D:501:HOH:O	2.06	0.55
1:D:238:THR:HG22	1:D:240:ALA:H	1.70	0.55
1:C:210:VAL:O	1:C:214:ILE:HG13	2.06	0.55
1:D:301:LEU:HB3	1:D:306:TYR:CD2	2.42	0.55
1:B:204:GLN:HA	2:B:538:HOH:O	2.06	0.55
1:D:415:ARG:HB2	1:C:415:ARG:CD	2.36	0.54
1:B:184:PRO:HB2	1:B:187:GLU:HG2	1.90	0.54
1:B:66:GLN:HG3	1:B:67:PRO:HD2	1.88	0.54
1:D:268:LYS:HD3	1:D:273:SER:HB2	1.89	0.53
1:D:271:PRO:HB3	1:D:321:VAL:HG11	1.91	0.53
1:C:65:LEU:HA	2:C:503:HOH:O	2.09	0.53
1:B:351:THR:O	1:B:355:GLN:HG3	2.09	0.53
1:A:56:LEU:HB2	1:A:95:LEU:HD22	1.91	0.53
1:C:244:LYS:HA	2:C:507:HOH:O	2.08	0.53
1:A:241:TYR:HB2	2:A:504:HOH:O	2.10	0.52
1:A:28:SER:HB3	1:A:39:LEU:HD11	1.90	0.52
1:D:106:PRO:HD2	2:D:604:HOH:O	2.07	0.52
1:B:241:TYR:HB2	2:B:502:HOH:O	2.08	0.52
1:A:14:THR:O	1:A:416:ILE:HG21	2.10	0.52
1:D:206:ILE:HG22	1:D:258:VAL:HG11	1.91	0.52
1:B:294:THR:HG21	2:B:533:HOH:O	2.10	0.52
1:D:357:ASN:HA	2:D:537:HOH:O	2.08	0.52
1:B:360:SER:HB2	1:B:366:VAL:O	2.09	0.52
1:A:416:ILE:HA	2:A:587:HOH:O	2.10	0.51
1:C:189:ILE:HD13	2:C:632:HOH:O	2.10	0.51
1:A:124:ILE:HD11	2:A:599:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ALA:HA	2:D:546:HOH:O	2.08	0.51
1:C:411:VAL:HG13	1:C:415:ARG:CZ	2.40	0.51
1:D:163:PRO:HG2	2:D:589:HOH:O	2.09	0.51
1:B:349:VAL:HG11	2:B:512:HOH:O	2.11	0.51
1:C:170:ASP:HB2	1:C:181:TYR:HE2	1.75	0.51
1:C:254:PRO:HG2	2:C:539:HOH:O	2.08	0.51
1:B:400:PHE:HA	2:B:624:HOH:O	2.11	0.51
1:B:78:VAL:HB	2:B:508:HOH:O	2.10	0.51
1:B:89:VAL:HB	1:B:124:ILE:HD13	1.93	0.51
1:C:38:THR:HG23	2:C:511:HOH:O	2.11	0.51
1:D:216:PHE:CD1	1:D:278:LEU:HG	2.46	0.51
1:D:341:GLN:HB3	1:D:397:VAL:HG22	1.93	0.51
1:C:307:ASP:O	1:C:311:ILE:HG13	2.11	0.50
1:A:405:GLU:OE2	1:A:405:GLU:HA	2.11	0.50
1:A:271:PRO:HB3	1:A:321:VAL:HG13	1.93	0.50
1:D:185:PHE:HB2	2:D:589:HOH:O	2.10	0.50
1:B:19:ILE:HD11	2:B:540:HOH:O	2.11	0.50
1:B:55:VAL:HG12	2:B:614:HOH:O	2.11	0.50
1:D:132:LEU:HD23	2:D:516:HOH:O	2.11	0.50
1:B:132:LEU:HD12	2:B:505:HOH:O	2.12	0.50
1:A:255:ILE:O	1:A:259:VAL:HG23	2.12	0.50
1:D:173:PRO:HG3	1:D:236:THR:HG21	1.93	0.50
1:B:144:ASN:O	1:B:145:LEU:HD23	2.11	0.50
1:A:132:LEU:HD13	2:A:593:HOH:O	2.10	0.49
1:A:40:TYR:HB3	1:A:43:LEU:HD11	1.94	0.49
1:A:157:LEU:HD11	1:B:368:LYS:HD2	1.95	0.49
1:A:342:VAL:HA	1:A:375:TYR:O	2.11	0.49
1:C:411:VAL:O	1:C:415:ARG:HG3	2.12	0.49
1:A:92:GLY:O	1:A:94:GLN:HG3	2.13	0.49
1:A:120:GLN:HB2	1:D:124:ILE:O	2.12	0.49
1:A:385:ILE:HB	2:A:509:HOH:O	2.13	0.49
1:B:101:ALA:HB1	1:B:250:ASN:HD22	1.77	0.49
1:D:322:PHE:HE1	2:D:522:HOH:O	1.95	0.49
1:C:51:VAL:HG23	2:C:562:HOH:O	2.12	0.49
1:D:293:MET:HE1	1:D:312:LEU:HD22	1.93	0.49
1:B:154:PHE:HA	2:B:563:HOH:O	2.13	0.49
1:C:67:PRO:HD3	1:C:296:TRP:CE3	2.48	0.49
1:D:290:PRO:O	1:D:291:ASP:HB3	2.13	0.48
1:B:87:THR:HB	1:B:122:GLU:HG2	1.94	0.48
1:B:210:VAL:HG21	2:B:584:HOH:O	2.13	0.48
1:B:299:LYS:HB3	2:B:641:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LYS:HD3	1:C:323:GLU:HG3	1.95	0.48
1:B:415:ARG:HH11	1:B:415:ARG:C	2.16	0.48
1:C:71:ARG:HD3	2:C:523:HOH:O	2.13	0.48
1:A:189:ILE:HB	2:A:502:HOH:O	2.13	0.48
1:A:162:VAL:O	1:A:328:VAL:HG13	2.14	0.48
1:B:212:ALA:HB2	2:B:503:HOH:O	2.14	0.48
1:B:55:VAL:HG13	2:B:518:HOH:O	2.13	0.48
1:A:288:GLN:HG2	1:A:289:CYS:N	2.29	0.48
1:A:366:VAL:HA	2:A:509:HOH:O	2.13	0.48
1:C:17:ARG:HG2	1:C:18:PRO:HD2	1.96	0.47
1:A:283:ASP:HA	1:A:295:GLN:HB2	1.95	0.47
1:D:38:THR:HG23	2:D:524:HOH:O	2.15	0.47
1:C:296:TRP:HZ3	2:C:503:HOH:O	1.97	0.47
1:D:253:GLU:HB3	1:D:254:PRO:HD3	1.96	0.47
1:D:284:GLY:HA3	1:D:294:THR:HG23	1.97	0.47
1:A:-6:ASN:HD22	1:A:-5:LEU:HD23	1.78	0.47
1:A:10:ILE:HG22	2:A:506:HOH:O	2.13	0.47
1:A:186:LYS:HA	2:A:613:HOH:O	2.14	0.47
1:A:263:PHE:HB2	2:A:613:HOH:O	2.15	0.47
1:A:293:MET:HE2	1:A:316:TYR:CE2	2.48	0.47
1:B:99:ILE:HG21	2:B:519:HOH:O	2.15	0.47
1:D:267:ILE:HG22	1:D:277:LEU:HB3	1.97	0.47
1:C:412:ALA:HB2	2:C:603:HOH:O	2.14	0.47
1:A:123:LEU:HD23	1:D:121:SER:HB3	1.97	0.47
1:A:186:LYS:HD2	2:A:558:HOH:O	2.15	0.47
1:D:207:TYR:CD2	1:D:262:ILE:HD13	2.50	0.47
1:A:360:SER:OG	1:A:368:LYS:HE2	2.15	0.47
1:D:157:LEU:HA	2:D:617:HOH:O	2.14	0.47
1:C:202:PRO:HD2	2:C:605:HOH:O	2.15	0.47
1:C:19:ILE:O	1:C:49:GLY:HA2	2.15	0.46
1:D:415:ARG:HB2	1:C:415:ARG:NE	2.30	0.46
1:B:408:ARG:HA	2:B:547:HOH:O	2.14	0.46
1:B:300:ASP:O	1:B:304:GLN:HG3	2.16	0.46
1:A:269:ARG:HG3	1:A:320:ILE:HG22	1.97	0.46
1:D:268:LYS:O	1:D:320:ILE:HA	2.15	0.46
1:A:86:GLU:HB3	2:A:540:HOH:O	2.14	0.46
1:A:130:HIS:CD2	1:A:132:LEU:HB2	2.50	0.46
1:D:259:VAL:HG13	2:D:626:HOH:O	2.15	0.46
1:B:90:ILE:HD13	1:B:103:GLN:NE2	2.31	0.46
1:B:142:GLU:HG2	1:B:146:LYS:NZ	2.31	0.46
1:B:169:HIS:HB2	1:B:233:PHE:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:HG22	2:A:501:HOH:O	2.15	0.46
1:C:90:ILE:HG21	1:C:103:GLN:NE2	2.30	0.46
1:A:190:LYS:N	2:A:502:HOH:O	2.49	0.46
1:C:312:LEU:HG	2:C:501:HOH:O	2.15	0.46
1:A:308:TYR:HD2	2:A:508:HOH:O	1.99	0.45
1:A:20:GLN:HG3	1:A:21:ASN:N	2.30	0.45
1:A:103:GLN:OE1	1:A:250:ASN:HB3	2.17	0.45
1:D:256:ASN:HB3	2:D:527:HOH:O	2.15	0.45
1:A:130:HIS:HD2	1:A:132:LEU:N	2.13	0.45
1:D:251:LEU:HD23	2:D:606:HOH:O	2.17	0.45
1:C:217:THR:HG22	2:C:540:HOH:O	2.15	0.45
1:A:201:TRP:HZ2	2:A:593:HOH:O	1.98	0.45
1:A:352:ILE:HD11	1:A:403:TRP:CE3	2.52	0.45
1:D:132:LEU:HD12	2:D:508:HOH:O	2.17	0.45
1:C:39:LEU:HD13	1:C:56:LEU:HD22	1.97	0.45
1:D:269:ARG:HB2	1:D:320:ILE:HG22	1.98	0.45
1:B:263:PHE:HA	2:B:634:HOH:O	2.16	0.45
1:A:99:ILE:HD13	1:A:99:ILE:HA	1.78	0.45
1:A:352:ILE:HD13	1:A:352:ILE:HA	1.68	0.45
1:D:294:THR:HG22	1:D:297:GLY:N	2.09	0.45
1:C:370:ILE:HD13	1:C:370:ILE:HA	1.90	0.45
1:D:62:ASP:HA	1:D:65:LEU:HD12	1.99	0.45
1:A:199:SER:HB3	1:A:255:ILE:HG13	1.99	0.44
1:A:239:THR:HG23	1:A:244:LYS:HB2	1.98	0.44
1:A:278:LEU:HD23	2:A:517:HOH:O	2.16	0.44
1:D:221:VAL:HG22	1:D:234:THR:HG21	1.99	0.44
1:A:122:GLU:HB2	2:A:599:HOH:O	2.17	0.44
1:B:40:TYR:HB3	1:B:43:LEU:HD11	1.99	0.44
1:B:339:THR:CG2	1:B:397:VAL:HG13	2.47	0.44
1:D:309:GLU:HB3	2:D:522:HOH:O	2.17	0.44
1:C:205:THR:O	1:C:208:ALA:HB3	2.16	0.44
1:B:217:THR:O	1:B:221:VAL:HG23	2.17	0.44
1:C:86:GLU:HA	1:C:110:ARG:CZ	2.48	0.44
1:C:196:GLU:HG2	2:C:537:HOH:O	2.16	0.44
1:D:339:THR:CG2	1:D:397:VAL:HG13	2.48	0.44
1:C:61:VAL:O	1:C:65:LEU:HD12	2.18	0.44
1:C:319:GLU:HG2	2:C:567:HOH:O	2.17	0.44
1:D:174:GLU:CD	1:D:174:GLU:H	2.21	0.44
1:C:185:PHE:HE1	2:C:540:HOH:O	2.00	0.44
1:C:199:SER:HB3	2:C:539:HOH:O	2.18	0.44
1:C:267:ILE:HD12	2:C:534:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:HB2	1:D:95:LEU:CD2	2.48	0.43
1:D:58:ALA:HA	1:D:74:SER:OG	2.18	0.43
1:D:99:ILE:HD12	1:D:254:PRO:HG2	2.00	0.43
1:B:259:VAL:HA	2:B:634:HOH:O	2.17	0.43
1:D:258:VAL:O	1:D:262:ILE:HG12	2.18	0.43
1:C:267:ILE:HG12	2:C:546:HOH:O	2.18	0.43
1:D:4:GLY:HA2	2:D:517:HOH:O	2.17	0.43
1:C:184:PRO:HD2	2:C:640:HOH:O	2.19	0.43
1:D:25:ASN:HB3	2:D:524:HOH:O	2.19	0.43
1:C:164:GLU:HB3	1:C:165:PHE:CD1	2.54	0.43
1:A:19:ILE:O	1:A:49:GLY:HA2	2.19	0.43
1:D:266:PHE:HB3	2:D:580:HOH:O	2.18	0.43
1:B:193:ALA:HB2	2:B:529:HOH:O	2.19	0.43
1:B:12:ASP:HB3	1:B:15:ASN:OD1	2.18	0.43
1:B:102:ARG:NH1	2:B:511:HOH:O	2.52	0.43
1:D:270:PRO:HG2	1:D:272:THR:HG22	2.02	0.42
1:B:280:GLN:O	1:B:292:GLN:HG2	2.19	0.42
1:A:260:ASP:HB3	1:A:401:LYS:HB2	2.01	0.42
1:A:384:LYS:HG3	1:A:396:GLY:CA	2.49	0.42
1:B:130:HIS:CD2	1:B:132:LEU:HB2	2.54	0.42
1:B:199:SER:HB2	2:B:504:HOH:O	2.18	0.42
1:B:206:ILE:HD13	1:B:206:ILE:HG21	1.77	0.42
1:A:271:PRO:HB3	1:A:321:VAL:CG1	2.49	0.42
1:B:119:ARG:NH1	1:C:178:ALA:HA	2.33	0.42
1:A:266:PHE:HE2	1:A:325:ALA:HB2	1.84	0.42
1:A:339:THR:HG23	1:A:397:VAL:HG13	2.01	0.42
1:D:298:SER:HB2	1:D:311:ILE:HG21	2.01	0.42
1:B:392:LEU:HB3	2:B:548:HOH:O	2.19	0.42
1:C:269:ARG:HA	2:C:567:HOH:O	2.19	0.42
1:A:89:VAL:HB	1:A:124:ILE:HD13	2.02	0.42
1:D:7:THR:HG22	2:D:514:HOH:O	2.18	0.42
1:D:162:VAL:O	1:D:328:VAL:HG12	2.19	0.42
1:B:242:ASP:N	2:B:502:HOH:O	2.52	0.42
1:A:207:TYR:HB2	2:A:508:HOH:O	2.19	0.42
1:C:288:GLN:HA	2:C:536:HOH:O	2.18	0.42
1:D:197:ILE:HG21	1:D:209:ASN:OD1	2.20	0.42
1:C:39:LEU:HA	1:C:39:LEU:HD23	1.84	0.42
1:C:299:LYS:HE2	1:C:303:ASP:OD1	2.19	0.42
1:B:38:THR:HG21	1:B:41:GLN:OE1	2.19	0.42
1:B:375:TYR:N	2:B:512:HOH:O	2.52	0.42
1:B:415:ARG:HB3	2:B:545:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:O	1:A:11:ILE:HG13	2.20	0.42
1:A:345:SER:HA	1:A:373:GLY:O	2.20	0.41
1:D:342:VAL:HG23	2:D:543:HOH:O	2.20	0.41
1:B:253:GLU:O	1:B:257:VAL:HG23	2.20	0.41
1:B:339:THR:HG23	1:B:397:VAL:HG13	2.02	0.41
1:C:190:LYS:HG3	2:C:518:HOH:O	2.19	0.41
1:D:281:TYR:HE2	2:D:590:HOH:O	2.01	0.41
1:C:218:LEU:HD23	1:C:218:LEU:HA	1.95	0.41
1:C:366:VAL:HA	2:C:538:HOH:O	2.19	0.41
1:C:169:HIS:HB2	1:C:233:PHE:CG	2.55	0.41
1:B:253:GLU:HG3	2:B:557:HOH:O	2.20	0.41
1:B:90:ILE:HB	2:B:508:HOH:O	2.21	0.41
1:C:170:ASP:HA	1:C:237:SER:OG	2.21	0.41
1:D:169:HIS:HE1	2:D:506:HOH:O	2.04	0.41
1:B:213:ILE:HG21	2:B:529:HOH:O	2.20	0.41
1:B:299:LYS:CB	2:B:641:HOH:O	2.68	0.41
1:C:22:ALA:O	1:C:44:ARG:HA	2.21	0.41
1:D:146:LYS:HD2	1:D:225:TRP:CZ3	2.55	0.41
1:D:160:PRO:HD3	1:D:274:ARG:O	2.21	0.41
1:B:157:LEU:HD13	2:B:648:HOH:O	2.19	0.41
1:C:410:TYR:O	1:C:414:THR:HB	2.20	0.41
1:D:87:THR:O	1:D:122:GLU:HB2	2.20	0.41
1:D:259:VAL:O	1:D:263:PHE:HB3	2.21	0.41
1:D:411:VAL:HG12	1:D:415:ARG:HD3	2.03	0.41
1:C:56:LEU:HB2	1:C:95:LEU:CD2	2.51	0.41
1:C:208:ALA:HA	2:C:501:HOH:O	2.21	0.41
1:D:132:LEU:HD11	1:D:201:TRP:CH2	2.56	0.41
1:B:262:ILE:HB	2:B:647:HOH:O	2.20	0.41
1:B:330:GLY:N	2:B:514:HOH:O	2.53	0.41
1:C:66:GLN:OE1	1:C:67:PRO:HD2	2.21	0.41
1:C:119:ARG:HD2	1:C:119:ARG:N	2.34	0.41
1:C:247:ASN:O	1:C:248:ASN:HB2	2.20	0.41
1:D:345:SER:HA	1:D:373:GLY:O	2.21	0.41
1:B:67:PRO:HG2	1:B:285:GLN:NE2	2.35	0.41
1:B:132:LEU:HA	1:B:132:LEU:HD23	1.76	0.41
1:B:255:ILE:HA	2:B:584:HOH:O	2.21	0.41
1:B:51:VAL:HB	2:B:665:HOH:O	2.21	0.40
1:B:372:ASP:OD2	1:B:374:ILE:HB	2.21	0.40
1:C:293:MET:HA	1:C:315:PHE:CD1	2.57	0.40
1:A:164:GLU:HB2	1:A:328:VAL:HG22	2.03	0.40
1:B:146:LYS:HD2	1:B:225:TRP:CZ3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ASN:HA	1:C:293:MET:HE1	2.04	0.40
1:D:293:MET:HE3	1:D:316:TYR:HE2	1.86	0.40
1:B:186:LYS:O	1:B:190:LYS:HG3	2.21	0.40
1:B:201:TRP:N	2:B:515:HOH:O	2.54	0.40
1:A:154:PHE:O	1:A:156:VAL:N	2.54	0.40
1:A:166:ILE:HG23	1:A:166:ILE:HD12	1.82	0.40
1:A:259:VAL:O	1:A:263:PHE:HB3	2.21	0.40
1:A:307:ASP:O	1:A:311:ILE:HG13	2.22	0.40
1:A:360:SER:HB2	1:A:366:VAL:O	2.21	0.40
1:D:20:GLN:HG3	1:D:46:ASN:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	406/480 (85%)	386 (95%)	19 (5%)	1 (0%)	44	45
1	B	404/480 (84%)	388 (96%)	14 (4%)	2 (0%)	25	23
1	C	400/480 (83%)	377 (94%)	22 (6%)	1 (0%)	37	37
1	D	398/480 (83%)	379 (95%)	16 (4%)	3 (1%)	16	13
All	All	1608/1920 (84%)	1530 (95%)	71 (4%)	7 (0%)	30	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-3	PHE
1	B	-4	TYR
1	A	-6	ASN
1	C	339	THR
1	D	42	ASN

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Mol	Chain	Res	Type
1	D	319	GLU
1	D	155	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	366/420 (87%)	347 (95%)	19 (5%)	19	18
1	B	365/420 (87%)	358 (98%)	7 (2%)	52	59
1	C	361/420 (86%)	349 (97%)	12 (3%)	33	36
1	D	359/420 (86%)	346 (96%)	13 (4%)	30	32
All	All	1451/1680 (86%)	1400 (96%)	51 (4%)	31	34

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	10	ILE
1	A	41	GLN
1	A	44	ARG
1	A	95	LEU
1	A	120	GLN
1	A	126	ASP
1	A	145	LEU
1	A	161	VAL
1	A	176	SER
1	A	199	SER
1	A	236	THR
1	A	243	HIS
1	A	272	THR
1	A	286	LYS
1	A	318	ASP
1	A	328	VAL
1	A	378	ASP
1	A	416	ILE

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Mol	Chain	Res	Type
1	D	29	MET
1	D	182	TRP
1	D	232	ASN
1	D	243	HIS
1	D	275	GLN
1	D	283	ASP
1	D	314	TYR
1	D	319	GLU
1	D	341	GLN
1	D	350	ARG
1	D	360	SER
1	D	378	ASP
1	D	397	VAL
1	B	-3	PHE
1	B	95	LEU
1	B	161	VAL
1	B	227	ARG
1	B	238	THR
1	B	243	HIS
1	B	281	TYR
1	C	39	LEU
1	C	95	LEU
1	C	139	LYS
1	C	227	ARG
1	C	236	THR
1	C	243	HIS
1	C	272	THR
1	C	285	GLN
1	C	328	VAL
1	C	360	SER
1	C	378	ASP
1	C	397	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	HIS
1	A	243	HIS
1	A	247	ASN
1	D	130	HIS
1	D	228	ASN
1	B	130	HIS

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Mol	Chain	Res	Type
1	B	243	HIS
1	C	144	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	412/480 (85%)	0.35	21 (5%)	34	36	31, 44, 71, 122	0
1	B	410/480 (85%)	0.35	13 (3%)	50	52	29, 43, 70, 110	0
1	C	406/480 (84%)	1.06	47 (11%)	11	11	37, 61, 94, 127	0
1	D	404/480 (84%)	0.79	36 (8%)	17	18	33, 55, 97, 127	0
All	All	1632/1920 (85%)	0.64	117 (7%)	23	25	29, 49, 88, 127	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-5	LEU	6.2
1	A	-5	LEU	5.7
1	B	-4	TYR	5.5
1	A	416	ILE	5.0
1	A	417	ALA	4.7
1	D	182	TRP	4.7
1	D	30	SER	4.4
1	A	415	ARG	4.3
1	D	156	VAL	4.2
1	B	182	TRP	3.9
1	D	154	PHE	3.8
1	C	154	PHE	3.8
1	D	293	MET	3.7
1	D	152	THR	3.7
1	D	312	LEU	3.7
1	C	30	SER	3.5
1	C	3	ASP	3.4
1	C	-1	GLY	3.4
1	C	281	TYR	3.3
1	B	154	PHE	3.2
1	C	66	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	-4	TYR	3.2
1	C	118	SER	3.1
1	D	205	THR	3.1
1	C	67	PRO	3.0
1	C	156	VAL	3.0
1	D	321	VAL	3.0
1	D	318	ASP	2.9
1	D	155	VAL	2.9
1	C	64	SER	2.9
1	D	272	THR	2.9
1	A	284	GLY	2.9
1	A	306	TYR	2.8
1	D	132	LEU	2.8
1	A	119	ARG	2.8
1	C	322	PHE	2.8
1	D	314	TYR	2.8
1	C	414	THR	2.8
1	D	271	PRO	2.8
1	C	308	TYR	2.8
1	C	61	VAL	2.8
1	B	189	ILE	2.7
1	C	134	GLY	2.7
1	C	182	TRP	2.7
1	A	290	PRO	2.6
1	A	232	ASN	2.6
1	B	118	SER	2.6
1	D	198	TYR	2.6
1	C	306	TYR	2.6
1	B	156	VAL	2.6
1	C	296	TRP	2.6
1	D	273	SER	2.6
1	D	70	VAL	2.6
1	D	199	SER	2.6
1	C	35	SER	2.6
1	D	300	ASP	2.5
1	B	318	ASP	2.5
1	C	283	ASP	2.5
1	A	155	VAL	2.5
1	C	216	PHE	2.5
1	A	287	SER	2.5
1	D	-1	GLY	2.5
1	C	279	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	293	MET	2.5
1	D	149	PRO	2.5
1	D	290	PRO	2.5
1	C	245	PHE	2.5
1	C	243	HIS	2.5
1	B	155	VAL	2.5
1	C	297	GLY	2.4
1	C	65	LEU	2.4
1	A	300	ASP	2.4
1	C	207	TYR	2.4
1	C	126	ASP	2.4
1	D	135	THR	2.4
1	C	135	THR	2.4
1	B	30	SER	2.3
1	D	281	TYR	2.3
1	C	290	PRO	2.2
1	C	303	ASP	2.2
1	D	39	LEU	2.2
1	D	218	LEU	2.2
1	C	172	LEU	2.2
1	A	285	GLN	2.2
1	A	182	TRP	2.2
1	D	267	ILE	2.2
1	D	35	SER	2.2
1	C	143	SER	2.2
1	B	290	PRO	2.2
1	D	289	CYS	2.2
1	D	241	TYR	2.2
1	C	227	ARG	2.2
1	C	98	THR	2.1
1	C	225	TRP	2.1
1	C	53	GLY	2.1
1	C	70	VAL	2.1
1	C	6	LEU	2.1
1	C	198	TYR	2.1
1	A	156	VAL	2.1
1	B	119	ARG	2.1
1	A	154	PHE	2.1
1	D	172	LEU	2.1
1	C	99	ILE	2.1
1	A	243	HIS	2.1
1	A	-1	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	138	PRO	2.1
1	D	225	TRP	2.1
1	C	119	ARG	2.1
1	A	64	SER	2.1
1	C	254	PRO	2.0
1	C	155	VAL	2.0
1	C	282	CYS	2.0
1	C	260	ASP	2.0
1	B	120	GLN	2.0
1	A	-3	PHE	2.0
1	D	279	ALA	2.0
1	D	415	ARG	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.