



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2026 – 04:22 pm BST

PDB ID : 9R6W / pdb\_00009r6w  
Title : CHAP domain of Pneumococcal Endopeptidase PcsB  
Authors : Briggs, N.S.; Roper, D.I.  
Deposited on : 2025-05-13  
Resolution : 1.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
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

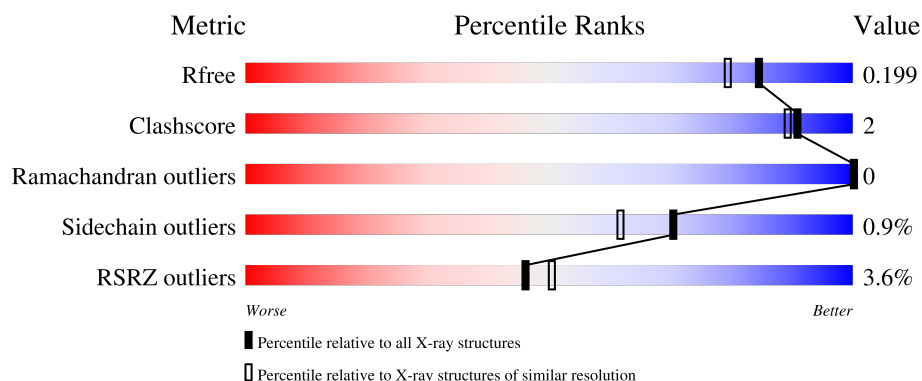
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	138	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 5%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: -10px; left: 5%; width: 75%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: -10px; left: 80%; width: 5%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: -10px; left: 85%; width: 10%; height: 10px; background-color: grey;"></div> </div> <div> <span style="display: inline-block; width: 5%; height: 10px; background-color: red; margin-right: 5px;"></span> <span style="display: inline-block; width: 75%; height: 10px; background-color: green; margin-right: 5px;"></span> <span style="display: inline-block; width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></span> <span style="display: inline-block; width: 10%; height: 10px; background-color: grey;"></span> </div> <div> <span style="display: inline-block; width: 5%; height: 10px; background-color: red; margin-right: 5px;"></span> <span style="display: inline-block; width: 75%; height: 10px; background-color: green; margin-right: 5px;"></span> <span style="display: inline-block; width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></span> <span style="display: inline-block; width: 10%; height: 10px; background-color: grey;"></span> </div> </div>
1	BBB	138	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 2%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: -10px; left: 2%; width: 76%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: -10px; left: 78%; width: 2%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: -10px; left: 80%; width: 12%; height: 10px; background-color: grey;"></div> </div> <div> <span style="display: inline-block; width: 2%; height: 10px; background-color: red; margin-right: 5px;"></span> <span style="display: inline-block; width: 76%; height: 10px; background-color: green; margin-right: 5px;"></span> <span style="display: inline-block; width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></span> <span style="display: inline-block; width: 12%; height: 10px; background-color: grey;"></span> </div> <div> <span style="display: inline-block; width: 2%; height: 10px; background-color: red; margin-right: 5px;"></span> <span style="display: inline-block; width: 76%; height: 10px; background-color: green; margin-right: 5px;"></span> <span style="display: inline-block; width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></span> <span style="display: inline-block; width: 12%; height: 10px; background-color: grey;"></span> </div> </div>
1	CCC	138	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 3%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: -10px; left: 3%; width: 78%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: -10px; left: 81%; width: 1%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: -10px; left: 82%; width: 16%; height: 10px; background-color: grey;"></div> </div> <div> <span style="display: inline-block; width: 3%; height: 10px; background-color: red; margin-right: 5px;"></span> <span style="display: inline-block; width: 78%; height: 10px; background-color: green; margin-right: 5px;"></span> <span style="display: inline-block; width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></span> <span style="display: inline-block; width: 16%; height: 10px; background-color: grey;"></span> </div> <div> <span style="display: inline-block; width: 3%; height: 10px; background-color: red; margin-right: 5px;"></span> <span style="display: inline-block; width: 78%; height: 10px; background-color: green; margin-right: 5px;"></span> <span style="display: inline-block; width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></span> <span style="display: inline-block; width: 16%; height: 10px; background-color: grey;"></span> </div> </div>
1	DDD	138	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 5%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: -10px; left: 5%; width: 75%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: -10px; left: 80%; width: 7%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: -10px; left: 87%; width: 18%; height: 10px; background-color: grey;"></div> </div> <div> <span style="display: inline-block; width: 5%; height: 10px; background-color: red; margin-right: 5px;"></span> <span style="display: inline-block; width: 75%; height: 10px; background-color: green; margin-right: 5px;"></span> <span style="display: inline-block; width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></span> <span style="display: inline-block; width: 18%; height: 10px; background-color: grey;"></span> </div> <div> <span style="display: inline-block; width: 5%; height: 10px; background-color: red; margin-right: 5px;"></span> <span style="display: inline-block; width: 75%; height: 10px; background-color: green; margin-right: 5px;"></span> <span style="display: inline-block; width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></span> <span style="display: inline-block; width: 18%; height: 10px; background-color: grey;"></span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3623 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 Peptidoglycan hydrolase PcsB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	108	Total	C	N	O	S	0	4	0
			838	526	145	165	2			
1	BBB	109	Total	C	N	O	S	0	3	0
			832	522	144	164	2			
1	CCC	110	Total	C	N	O	S	0	1	0
			826	519	144	161	2			
1	DDD	112	Total	C	N	O	S	0	0	0
			840	529	145	164	2			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-5	MET	-	initiating methionine	UNP A0A0H2ZQ76
AAA	-4	GLY	-	expression tag	UNP A0A0H2ZQ76
AAA	-3	SER	-	expression tag	UNP A0A0H2ZQ76
AAA	-2	SER	-	expression tag	UNP A0A0H2ZQ76
AAA	-1	HIS	-	expression tag	UNP A0A0H2ZQ76
AAA	0	HIS	-	expression tag	UNP A0A0H2ZQ76
AAA	1	HIS	-	expression tag	UNP A0A0H2ZQ76
AAA	2	HIS	-	expression tag	UNP A0A0H2ZQ76
AAA	3	HIS	-	expression tag	UNP A0A0H2ZQ76
AAA	4	HIS	-	expression tag	UNP A0A0H2ZQ76
AAA	5	SER	-	expression tag	UNP A0A0H2ZQ76
AAA	6	SER	-	expression tag	UNP A0A0H2ZQ76
AAA	7	GLY	-	expression tag	UNP A0A0H2ZQ76
AAA	8	LEU	-	expression tag	UNP A0A0H2ZQ76
AAA	9	VAL	-	expression tag	UNP A0A0H2ZQ76
AAA	10	PRO	-	expression tag	UNP A0A0H2ZQ76
AAA	11	ARG	-	expression tag	UNP A0A0H2ZQ76
AAA	12	GLY	-	expression tag	UNP A0A0H2ZQ76
AAA	13	SER	-	expression tag	UNP A0A0H2ZQ76
BBB	-5	MET	-	initiating methionine	UNP A0A0H2ZQ76
BBB	-4	GLY	-	expression tag	UNP A0A0H2ZQ76

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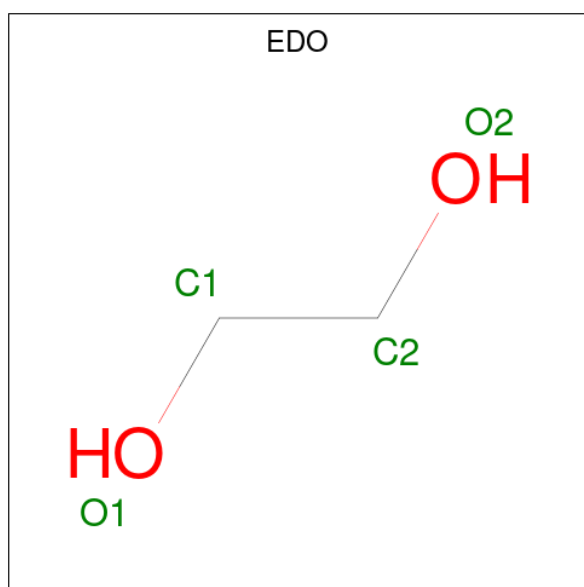
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-3	SER	-	expression tag	UNP A0A0H2ZQ76
BBB	-2	SER	-	expression tag	UNP A0A0H2ZQ76
BBB	-1	HIS	-	expression tag	UNP A0A0H2ZQ76
BBB	0	HIS	-	expression tag	UNP A0A0H2ZQ76
BBB	1	HIS	-	expression tag	UNP A0A0H2ZQ76
BBB	2	HIS	-	expression tag	UNP A0A0H2ZQ76
BBB	3	HIS	-	expression tag	UNP A0A0H2ZQ76
BBB	4	HIS	-	expression tag	UNP A0A0H2ZQ76
BBB	5	SER	-	expression tag	UNP A0A0H2ZQ76
BBB	6	SER	-	expression tag	UNP A0A0H2ZQ76
BBB	7	GLY	-	expression tag	UNP A0A0H2ZQ76
BBB	8	LEU	-	expression tag	UNP A0A0H2ZQ76
BBB	9	VAL	-	expression tag	UNP A0A0H2ZQ76
BBB	10	PRO	-	expression tag	UNP A0A0H2ZQ76
BBB	11	ARG	-	expression tag	UNP A0A0H2ZQ76
BBB	12	GLY	-	expression tag	UNP A0A0H2ZQ76
BBB	13	SER	-	expression tag	UNP A0A0H2ZQ76
CCC	-5	MET	-	initiating methionine	UNP A0A0H2ZQ76
CCC	-4	GLY	-	expression tag	UNP A0A0H2ZQ76
CCC	-3	SER	-	expression tag	UNP A0A0H2ZQ76
CCC	-2	SER	-	expression tag	UNP A0A0H2ZQ76
CCC	-1	HIS	-	expression tag	UNP A0A0H2ZQ76
CCC	0	HIS	-	expression tag	UNP A0A0H2ZQ76
CCC	1	HIS	-	expression tag	UNP A0A0H2ZQ76
CCC	2	HIS	-	expression tag	UNP A0A0H2ZQ76
CCC	3	HIS	-	expression tag	UNP A0A0H2ZQ76
CCC	4	HIS	-	expression tag	UNP A0A0H2ZQ76
CCC	5	SER	-	expression tag	UNP A0A0H2ZQ76
CCC	6	SER	-	expression tag	UNP A0A0H2ZQ76
CCC	7	GLY	-	expression tag	UNP A0A0H2ZQ76
CCC	8	LEU	-	expression tag	UNP A0A0H2ZQ76
CCC	9	VAL	-	expression tag	UNP A0A0H2ZQ76
CCC	10	PRO	-	expression tag	UNP A0A0H2ZQ76
CCC	11	ARG	-	expression tag	UNP A0A0H2ZQ76
CCC	12	GLY	-	expression tag	UNP A0A0H2ZQ76
CCC	13	SER	-	expression tag	UNP A0A0H2ZQ76
DDD	-5	MET	-	initiating methionine	UNP A0A0H2ZQ76
DDD	-4	GLY	-	expression tag	UNP A0A0H2ZQ76
DDD	-3	SER	-	expression tag	UNP A0A0H2ZQ76
DDD	-2	SER	-	expression tag	UNP A0A0H2ZQ76
DDD	-1	HIS	-	expression tag	UNP A0A0H2ZQ76
DDD	0	HIS	-	expression tag	UNP A0A0H2ZQ76

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	1	HIS	-	expression tag	UNP A0A0H2ZQ76
DDD	2	HIS	-	expression tag	UNP A0A0H2ZQ76
DDD	3	HIS	-	expression tag	UNP A0A0H2ZQ76
DDD	4	HIS	-	expression tag	UNP A0A0H2ZQ76
DDD	5	SER	-	expression tag	UNP A0A0H2ZQ76
DDD	6	SER	-	expression tag	UNP A0A0H2ZQ76
DDD	7	GLY	-	expression tag	UNP A0A0H2ZQ76
DDD	8	LEU	-	expression tag	UNP A0A0H2ZQ76
DDD	9	VAL	-	expression tag	UNP A0A0H2ZQ76
DDD	10	PRO	-	expression tag	UNP A0A0H2ZQ76
DDD	11	ARG	-	expression tag	UNP A0A0H2ZQ76
DDD	12	GLY	-	expression tag	UNP A0A0H2ZQ76
DDD	13	SER	-	expression tag	UNP A0A0H2ZQ76

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	BBB	1	Total	C	O	0	0
			4	2	2		
2	BBB	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	CCC	1	Total	C	O	0	0
			4	2	2		
2	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Ca	0	0
			1	1		

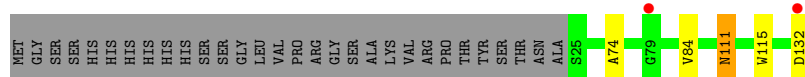
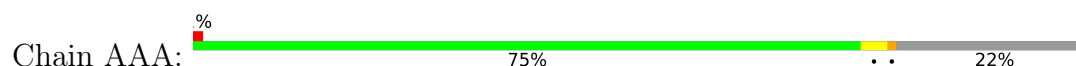
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	56	Total	O	0	0
			56	56		
4	BBB	84	Total	O	0	0
			84	84		
4	CCC	64	Total	O	0	0
			64	64		
4	DDD	54	Total	O	0	0
			54	54		

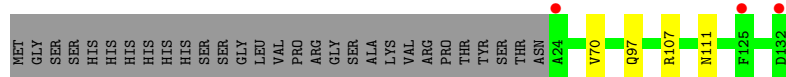
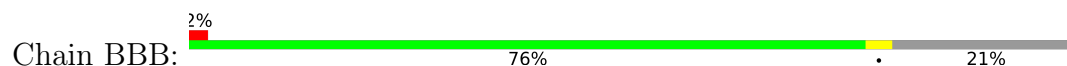
### 3 Residue-property plots [i](#)

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.

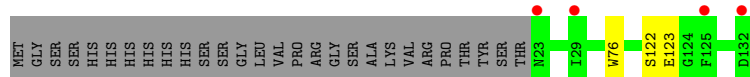
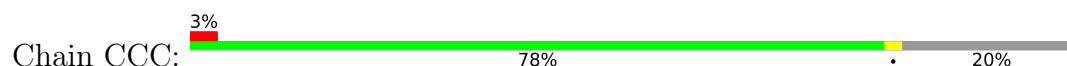
- Molecule 1: Peptidoglycan hydrolase PcsB



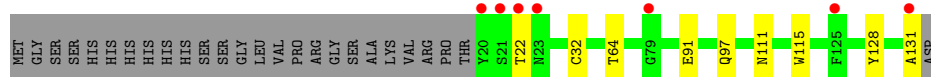
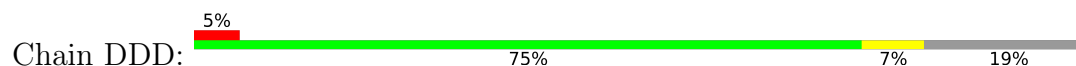
- Molecule 1: Peptidoglycan hydrolase PcsB



- Molecule 1: Peptidoglycan hydrolase PcsB



- Molecule 1: Peptidoglycan hydrolase PcsB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.28Å 117.38Å 47.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.22 – 1.70 44.22 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.22-1.70) 100.0 (44.22-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.27 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.172 , 0.194 0.183 , 0.199	Depositor DCC
$R_{free}$ test set	2634 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 25.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	AAA	0.99	0/864	1.14	1/1186 (0.1%)
1	BBB	1.12	1/861 (0.1%)	1.18	0/1182
1	CCC	1.09	0/852	1.19	0/1170
1	DDD	1.07	0/867	1.25	3/1191 (0.3%)
All	All	1.07	1/3444 (0.0%)	1.19	4/4729 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	70	VAL	C-O	5.78	1.30	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	131	ALA	CA-C-O	-11.53	101.20	120.80
1	DDD	32	CYS	CA-C-N	5.26	127.28	120.44
1	DDD	32	CYS	C-N-CA	5.26	127.28	120.44
1	AAA	132	ASP	CA-C-O	5.06	129.40	120.80

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	AAA	838	0	757	3	0
1	BBB	832	0	756	2	0
1	CCC	826	0	750	1	0
1	DDD	840	0	765	6	0
2	AAA	12	0	18	0	0
2	BBB	8	0	12	0	0
2	CCC	4	0	6	0	0
2	DDD	4	0	6	0	0
3	AAA	1	0	0	0	0
4	AAA	56	0	0	0	0
4	BBB	84	0	0	0	0
4	CCC	64	0	0	0	0
4	DDD	54	0	0	0	0
All	All	3623	0	3070	11	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 (11) 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:DDD:91:GLU:HG3	1:DDD:115:TRP:CH2	2.38	0.58
1:BBB:97:GLN:NE2	1:BBB:111:ASN:HD21	2.06	0.53
1:BBB:97:GLN:HE21	1:BBB:111:ASN:HD21	1.58	0.51
1:DDD:91:GLU:HG3	1:DDD:115:TRP:CZ3	2.47	0.49
1:DDD:97:GLN:NE2	1:DDD:111:ASN:HD21	2.10	0.48
1:DDD:97:GLN:HE21	1:DDD:111:ASN:HD21	1.60	0.48
1:AAA:111:ASN:C	1:AAA:111:ASN:HD22	2.23	0.45
1:DDD:64:THR:HA	1:DDD:128:TYR:O	2.17	0.43
1:CCC:76:TRP:HB3	1:CCC:123:GLU:O	2.19	0.43
1:AAA:74:ALA:O	1:AAA:84:VAL:HA	2.20	0.42
1:AAA:115:TRP:CD1	1:DDD:22:THR:HG21	2.55	0.41

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	AAA	110/138 (80%)	106 (96%)	4 (4%)	0	100	100
1	BBB	110/138 (80%)	109 (99%)	1 (1%)	0	100	100
1	CCC	109/138 (79%)	107 (98%)	2 (2%)	0	100	100
1	DDD	110/138 (80%)	108 (98%)	2 (2%)	0	100	100
All	All	439/552 (80%)	430 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	82/104 (79%)	81 (99%)	1 (1%)	63	51
1	BBB	82/104 (79%)	81 (99%)	1 (1%)	63	51
1	CCC	80/104 (77%)	78 (98%)	2 (2%)	42	24
1	DDD	82/104 (79%)	82 (100%)	0	100	100
All	All	326/416 (78%)	322 (99%)	4 (1%)	70	51

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	111	ASN
1	BBB	107	ARG
1	CCC	122[A]	SER
1	CCC	122[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EDO	AAA	202	-	3,3,3	0.31	0	2,2,2	0.42	0
2	EDO	BBB	201	-	3,3,3	0.20	0	2,2,2	0.07	0
2	EDO	BBB	202	-	3,3,3	0.13	0	2,2,2	0.24	0
2	EDO	AAA	201	-	3,3,3	0.15	0	2,2,2	0.21	0
2	EDO	AAA	203	-	3,3,3	0.23	0	2,2,2	0.10	0
2	EDO	DDD	201	-	3,3,3	0.37	0	2,2,2	0.06	0
2	EDO	CCC	201	-	3,3,3	0.45	0	2,2,2	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	AAA	202	-	-	0/1/1/1	-
2	EDO	BBB	201	-	-	0/1/1/1	-
2	EDO	BBB	202	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	AAA	201	-	-	0/1/1/1	-
2	EDO	AAA	203	-	-	0/1/1/1	-
2	EDO	DDD	201	-	-	1/1/1/1	-
2	EDO	CCC	201	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	CCC	201	EDO	O1-C1-C2-O2
2	DDD	201	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	AAA	108/138 (78%)	-0.11	2 (1%)	66	71	8, 17, 28, 44	4 (3%)
1	BBB	109/138 (78%)	-0.10	3 (2%)	55	59	8, 18, 27, 49	3 (2%)
1	CCC	110/138 (79%)	-0.00	4 (3%)	46	50	10, 19, 31, 45	1 (0%)
1	DDD	112/138 (81%)	0.12	7 (6%)	26	28	14, 19, 32, 45	0
All	All	439/552 (79%)	-0.02	16 (3%)	46	50	8, 18, 30, 49	8 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	22	THR	3.9
1	DDD	20	TYR	3.8
1	DDD	79	GLY	3.6
1	CCC	23	ASN	3.4
1	BBB	132	ASP	3.3
1	DDD	21	SER	3.2
1	BBB	125	PHE	2.7
1	AAA	132	ASP	2.5
1	DDD	131	ALA	2.5
1	DDD	23	ASN	2.5
1	CCC	132	ASP	2.5
1	CCC	125	PHE	2.4
1	CCC	29	ILE	2.4
1	BBB	24	ALA	2.3
1	DDD	125	PHE	2.3
1	AAA	79	GLY	2.2

### 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 [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	AAA	203	4/4	0.89	0.17	40,41,45,47	0
3	CA	AAA	204	1/1	0.91	0.25	52,52,52,52	0
2	EDO	BBB	202	4/4	0.93	0.13	19,20,21,22	0
2	EDO	AAA	202	4/4	0.93	0.11	22,24,24,25	0
2	EDO	DDD	201	4/4	0.96	0.07	21,21,21,22	0
2	EDO	AAA	201	4/4	0.97	0.06	18,19,19,20	0
2	EDO	BBB	201	4/4	0.98	0.04	16,17,18,18	0
2	EDO	CCC	201	4/4	0.98	0.05	19,20,20,20	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.