



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 05:38 AM EST

PDB ID : 5VNX  
Title : Crystal structure of an 8-amino-7-oxononanoate synthase from *Burkholderia multivorans* with a potential glycine-PLP-Lys242 cyclized intermediate or byproduct  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2017-05-01  
Resolution : 1.65 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

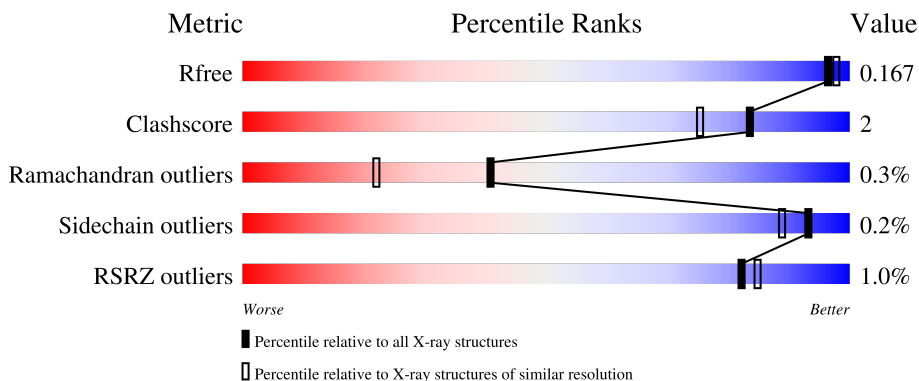
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	A	393	 96%
1	B	393	 93% 6%
1	C	393	 94% 5%

## 2 Entry composition [i](#)

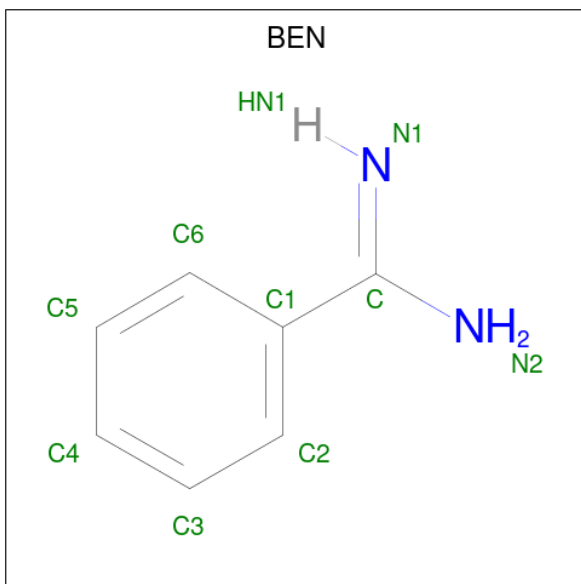
There are 5 unique types of molecules in this entry. The entry contains 10651 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 8-amino-7-oxononanoate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	393	Total 3009	C 1894	N 540	O 566	P 1	S 8	0	22	0
1	B	392	Total 3041	C 1911	N 550	O 572	P 1	S 7	0	25	0
1	C	392	Total 3064	C 1923	N 556	O 577	P 1	S 7	0	28	0

- Molecule 2 is BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



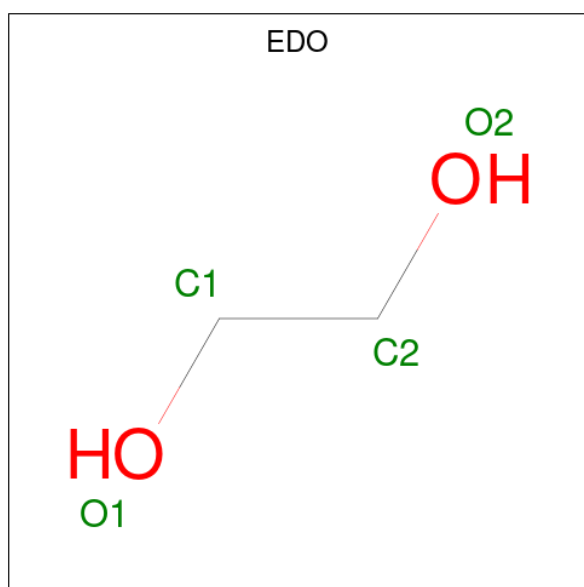
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	Total 9	C 7	N 2	0	0
2	A	1	Total 9	C 7	N 2	0	0
2	B	1	Total 9	C 7	N 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	N	0	0
			9	7	2		
2	C	1	Total	C	N	0	0
			9	7	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

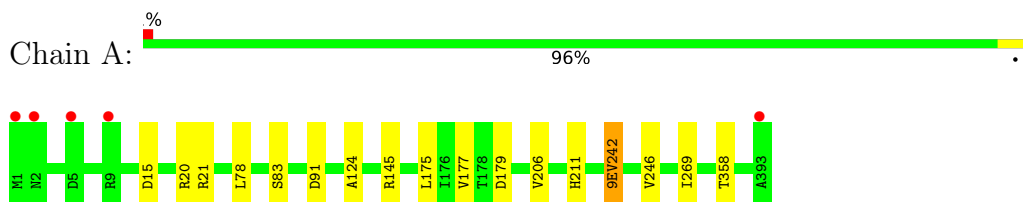
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	485	Total O 501 501	0	18
5	B	494	Total O 505 505	0	15
5	C	434	Total O 439 439	0	9

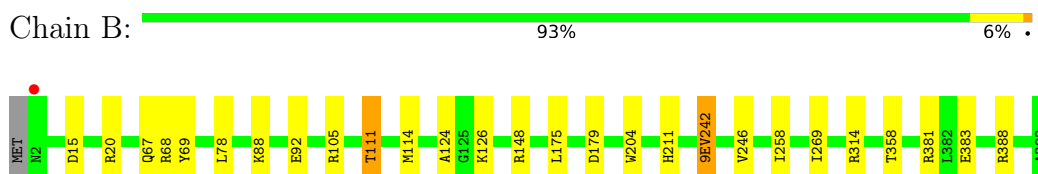
### 3 Residue-property plots [i](#)

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.

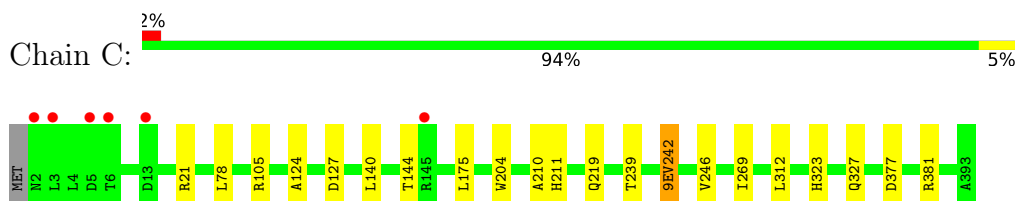
- Molecule 1: 8-amino-7-oxonanoate synthase



- Molecule 1: 8-amino-7-oxonanoate synthase



- Molecule 1: 8-amino-7-oxonanoate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.53Å 262.09Å 65.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.38 – 1.65 48.99 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.38-1.65) 100.0 (48.99-1.65)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 1.65Å)	Xtrriage
Refinement program	PHENIX dev_2733	Depositor
R, $R_{free}$	0.146 , 0.167 0.146 , 0.167	Depositor DCC
$R_{free}$ test set	2011 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9EV, SO4, BEN, 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	A	0.55	0/3084	0.72	1/4202 (0.0%)
1	B	0.52	0/3110	0.71	2/4235 (0.0%)
1	C	0.47	0/3126	0.67	0/4257
All	All	0.52	0/9320	0.70	3/12694 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	388	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	179	ASP	CB-CG-OD1	5.54	123.28	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3009	0	2978	13	0
1	B	3041	0	3005	17	0
1	C	3064	0	3032	13	0
2	A	18	0	14	2	0
2	B	18	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	9	0	7	1	0
3	A	12	0	18	0	0
3	B	8	0	12	1	0
3	C	12	0	18	0	0
4	A	5	0	0	0	0
4	C	10	0	0	0	0
5	A	501	0	0	3	0
5	B	505	0	0	7	0
5	C	439	0	0	5	1
All	All	10651	0	9098	44	1

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 (44) 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:A:175[B]:LEU:HD21	1:A:177[B]:VAL:HG13	1.64	0.80
1:B:314[B]:ARG:NH1	1:B:383:GLU:OE2	2.21	0.74
1:C:127[A]:ASP:OD2	5:C:701:HOH:O	2.10	0.69
1:B:15:ASP:OD2	5:B:701[A]:HOH:O	2.13	0.66
1:B:78[A]:LEU:HD22	1:B:269:ILE:HG12	1.76	0.66
1:A:175[B]:LEU:CD2	1:A:177[B]:VAL:HG13	2.29	0.63
1:B:381:ARG:NH2	5:B:702:HOH:O	2.14	0.63
1:C:219:GLN:NE2	5:C:702:HOH:O	2.21	0.62
1:A:78[A]:LEU:HD22	1:A:269:ILE:HG12	1.80	0.62
1:C:323:HIS:ND1	5:C:705:HOH:O	2.31	0.59
1:C:78[A]:LEU:HD22	1:C:269:ILE:HG12	1.84	0.58
1:C:21:ARG:HH21	2:C:601:BEN:HN22	1.52	0.58
1:C:211:HIS:NE2	1:C:242:9EV:O29	2.34	0.57
1:B:67[A]:GLN:NE2	5:B:706:HOH:O	2.37	0.56
1:B:20:ARG:NH1	5:B:703:HOH:O	2.28	0.56
1:C:105[B]:ARG:HD3	5:C:948:HOH:O	2.05	0.56
1:A:21:ARG:HH21	2:A:601:BEN:HN22	1.55	0.54
1:A:91:ASP:OD1	5:A:701[A]:HOH:O	2.19	0.54
1:B:211:HIS:NE2	1:B:242:9EV:O29	2.36	0.53
1:C:140:LEU:O	1:C:144:THR:HG23	2.09	0.53
1:A:211:HIS:NE2	1:A:242:9EV:O29	2.39	0.51
1:A:177[B]:VAL:HG12	1:A:206:VAL:HB	1.91	0.51
1:C:210:ALA:HA	1:C:239[B]:THR:HG22	1.94	0.49
1:B:111[B]:THR:OG1	1:B:114[B]:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175[B]:LEU:HD13	1:C:204:TRP:HB2	1.96	0.48
1:A:15[A]:ASP:OD1	1:A:20:ARG:HD2	2.14	0.47
1:B:88[B]:LYS:HG3	5:B:1005:HOH:O	2.15	0.46
1:C:381:ARG:NH1	5:C:707:HOH:O	2.35	0.46
1:B:358:THR:HG21	2:B:601:BEN:H2	2.00	0.44
3:B:604:EDO:H12	5:B:1100:HOH:O	2.16	0.44
1:B:126[B]:LYS:HA	1:B:148[B]:ARG:O	2.18	0.44
1:A:124:ALA:HB2	1:A:175[A]:LEU:HD13	2.00	0.43
1:B:88[B]:LYS:HG2	1:B:92:GLU:OE2	2.19	0.43
1:A:145[B]:ARG:HG3	5:A:834:HOH:O	2.19	0.43
1:C:312[B]:LEU:HD11	1:C:327:GLN:HB3	2.01	0.43
1:C:124:ALA:HB2	1:C:175[B]:LEU:HG	2.01	0.42
1:B:68:ARG:HD2	1:B:69[A]:TYR:CE2	2.54	0.42
1:B:124:ALA:HB2	1:B:175[B]:LEU:HD13	2.02	0.41
2:B:601:BEN:H4	5:B:1008[B]:HOH:O	2.19	0.41
1:A:21:ARG:HG2	1:B:78[A]:LEU:HD23	2.03	0.41
1:B:175[B]:LEU:HG	1:B:204:TRP:HB2	2.02	0.41
1:A:83:SER:HB2	5:A:819:HOH:O	2.19	0.41
1:A:358:THR:HG21	2:A:601:BEN:H6	2.03	0.41
1:B:105[B]:ARG:HB3	1:B:258:ILE:HG13	2.02	0.40

All (1) 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)
5:C:986:HOH:O	5:C:1003:HOH:O[4_556]	2.07	0.13

## 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	412/393 (105%)	404 (98%)	7 (2%)	1 (0%)	47 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	414/393 (105%)	401 (97%)	12 (3%)	1 (0%)	47	28
1	C	417/393 (106%)	409 (98%)	7 (2%)	1 (0%)	47	28
All	All	1243/1179 (105%)	1214 (98%)	26 (2%)	3 (0%)	41	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	VAL
1	B	246	VAL
1	C	246	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	295/283 (104%)	295 (100%)	0	100	100
1	B	298/283 (105%)	296 (99%)	2 (1%)	84	73
1	C	302/283 (107%)	301 (100%)	1 (0%)	92	88
All	All	895/849 (105%)	892 (100%)	3 (0%)	93	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	111[A]	THR
1	B	111[B]	THR
1	C	377	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	152	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](#)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	9EV	A	242	1	26,29,30	1.80	2 (7%)	29,41,43	3.97	7 (24%)
1	9EV	B	242	1	26,29,30	1.92	3 (11%)	29,41,43	3.79	8 (27%)
1	9EV	C	242	1	26,29,30	1.76	4 (15%)	29,41,43	3.47	9 (31%)

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
1	9EV	A	242	1	-	3/18/31/33	0/2/2/2
1	9EV	B	242	1	-	4/18/31/33	0/2/2/2
1	9EV	C	242	1	-	6/18/31/33	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	242	9EV	O14-C15	6.96	1.46	1.35
1	A	242	9EV	O14-C15	6.33	1.45	1.35
1	C	242	9EV	O14-C15	5.70	1.44	1.35
1	B	242	9EV	C01-C02	3.39	1.56	1.50
1	A	242	9EV	C01-C02	3.37	1.56	1.50
1	C	242	9EV	C01-C02	2.74	1.55	1.50
1	C	242	9EV	C17-C15	-2.19	1.45	1.51
1	B	242	9EV	C28-C02	-2.15	1.38	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	242	9EV	O14-C13	-2.02	1.41	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	9EV	O14-C13-N18	12.87	112.24	103.25
1	A	242	9EV	O14-C13-N18	11.99	111.62	103.25
1	A	242	9EV	C13-O14-C15	-11.89	101.03	111.85
1	B	242	9EV	C13-O14-C15	-11.67	101.23	111.85
1	C	242	9EV	C13-O14-C15	-11.29	101.57	111.85
1	C	242	9EV	O14-C13-N18	10.56	110.62	103.25
1	A	242	9EV	O14-C13-C12	6.73	116.66	109.18
1	A	242	9EV	O14-C15-O16	6.59	127.16	120.79
1	B	242	9EV	O14-C15-O16	6.56	127.13	120.79
1	A	242	9EV	O14-C15-C17	6.16	113.79	110.03
1	C	242	9EV	O14-C15-O16	5.58	126.19	120.79
1	C	242	9EV	C19-N18-C13	-4.26	106.54	114.11
1	A	242	9EV	C19-N18-C13	-4.15	106.73	114.11
1	B	242	9EV	O14-C13-C12	3.91	113.53	109.18
1	C	242	9EV	O14-C15-C17	3.85	112.38	110.03
1	B	242	9EV	O14-C15-C17	3.06	111.89	110.03
1	B	242	9EV	C19-N18-C13	-2.95	108.86	114.11
1	B	242	9EV	O11-P08-O07	-2.56	99.92	106.73
1	B	242	9EV	C05-C04-N03	-2.50	119.65	123.82
1	C	242	9EV	C05-C04-N03	-2.40	119.82	123.82
1	C	242	9EV	C06-C05-C12	-2.35	118.94	122.82
1	C	242	9EV	C20-C21-C22	2.32	121.84	113.62
1	C	242	9EV	O11-P08-O07	-2.22	100.83	106.73
1	A	242	9EV	C06-C05-C12	-2.21	119.17	122.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	242	9EV	O-C-CA-C22
1	B	242	9EV	C12-C05-C06-O07
1	B	242	9EV	O-C-CA-C22
1	C	242	9EV	O-C-CA-C22
1	C	242	9EV	N18-C19-C20-C21
1	A	242	9EV	N18-C19-C20-C21
1	B	242	9EV	N18-C19-C20-C21
1	A	242	9EV	C04-C05-C06-O07

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Mol	Chain	Res	Type	Atoms
1	B	242	9EV	C04-C05-C06-O07
1	C	242	9EV	C04-C05-C06-O07
1	C	242	9EV	C12-C05-C06-O07
1	C	242	9EV	C20-C19-N18-C13
1	C	242	9EV	C20-C19-N18-C17

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	242	9EV	1	0
1	B	242	9EV	1	0
1	C	242	9EV	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	BEN	B	602	-	9,9,9	1.41	1 (11%)	7,11,11	0.99	1 (14%)
2	BEN	C	601	-	9,9,9	1.19	1 (11%)	7,11,11	1.17	1 (14%)
3	EDO	C	605	-	3,3,3	0.41	0	2,2,2	0.46	0
2	BEN	A	602	-	9,9,9	1.33	1 (11%)	7,11,11	1.23	1 (14%)
3	EDO	C	604	-	3,3,3	0.51	0	2,2,2	0.34	0
4	SO4	A	605	-	4,4,4	0.13	0	6,6,6	0.14	0
4	SO4	C	602	-	4,4,4	0.14	0	6,6,6	0.14	0
3	EDO	B	603	-	3,3,3	0.44	0	2,2,2	0.27	0
3	EDO	C	606	-	3,3,3	0.40	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	604	-	3,3,3	0.49	0	2,2,2	0.55	0
2	BEN	B	601	-	9,9,9	1.28	1 (11%)	7,11,11	1.18	1 (14%)
4	SO4	C	603	-	4,4,4	0.14	0	6,6,6	0.10	0
3	EDO	A	606	-	3,3,3	0.49	0	2,2,2	0.42	0
3	EDO	A	603	-	3,3,3	0.41	0	2,2,2	0.17	0
3	EDO	B	604	-	3,3,3	0.53	0	2,2,2	0.14	0
2	BEN	A	601	-	9,9,9	1.25	1 (11%)	7,11,11	0.66	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	BEN	B	602	-	-	4/4/4/4	0/1/1/1
2	BEN	C	601	-	-	1/4/4/4	0/1/1/1
3	EDO	C	605	-	-	1/1/1/1	-
2	BEN	A	602	-	-	4/4/4/4	0/1/1/1
3	EDO	C	604	-	-	1/1/1/1	-
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	C	606	-	-	0/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
2	BEN	B	601	-	-	1/4/4/4	0/1/1/1
3	EDO	A	606	-	-	1/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
3	EDO	B	604	-	-	1/1/1/1	-
2	BEN	A	601	-	-	0/4/4/4	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	BEN	C1-C	-3.85	1.40	1.47
2	A	602	BEN	C1-C	-3.64	1.40	1.47
2	A	601	BEN	C1-C	-3.31	1.41	1.47
2	B	601	BEN	C1-C	-3.26	1.41	1.47
2	C	601	BEN	C1-C	-3.05	1.41	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	BEN	C1-C-N2	2.52	121.85	118.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	BEN	C1-C-N2	2.46	121.76	118.05
2	B	601	BEN	C1-C-N2	2.40	121.67	118.05
2	B	602	BEN	C1-C-N2	2.33	121.55	118.05

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	604	EDO	O1-C1-C2-O2
3	C	604	EDO	O1-C1-C2-O2
3	A	606	EDO	O1-C1-C2-O2
2	A	602	BEN	N2-C-C1-C2
2	A	602	BEN	N2-C-C1-C6
2	B	602	BEN	N2-C-C1-C2
2	B	602	BEN	N2-C-C1-C6
3	C	605	EDO	O1-C1-C2-O2
2	A	602	BEN	N1-C-C1-C2
2	A	602	BEN	N1-C-C1-C6
2	B	601	BEN	N1-C-C1-C6
2	B	602	BEN	N1-C-C1-C2
2	B	602	BEN	N1-C-C1-C6
2	C	601	BEN	N1-C-C1-C6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	BEN	1	0
2	B	601	BEN	2	0
3	B	604	EDO	1	0
2	A	601	BEN	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	A	392/393 (99%)	-0.31	5 (1%) 77 80	11, 17, 33, 73	0
1	B	391/393 (99%)	-0.45	1 (0%) 94 94	13, 19, 36, 61	0
1	C	391/393 (99%)	-0.27	6 (1%) 73 77	14, 20, 37, 63	0
All	All	1174/1179 (99%)	-0.35	12 (1%) 82 85	11, 19, 36, 73	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.1
1	C	145[A]	ARG	3.4
1	C	5	ASP	2.9
1	C	2	ASN	2.7
1	C	13	ASP	2.5
1	C	6	THR	2.5
1	B	2	ASN	2.4
1	A	2	ASN	2.3
1	C	3	LEU	2.3
1	A	9	ARG	2.3
1	A	5	ASP	2.1
1	A	393	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	9EV	B	242	28/29	0.94	0.10	14,19,26,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	9EV	C	242	28/29	0.94	0.10	13,22,31,32	0
1	9EV	A	242	28/29	0.95	0.09	12,18,24,27	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	A	605	5/5	0.58	0.28	102,105,107,114	0
3	EDO	A	604	4/4	0.79	0.15	40,47,48,57	0
2	BEN	A	602	9/9	0.80	0.21	34,40,54,59	0
2	BEN	B	602	9/9	0.83	0.25	33,44,51,57	0
3	EDO	A	606	4/4	0.85	0.14	47,51,52,55	0
3	EDO	B	603	4/4	0.87	0.11	49,54,56,59	0
4	SO4	C	602	5/5	0.87	0.23	113,113,115,116	0
3	EDO	C	604	4/4	0.88	0.15	35,48,49,56	0
3	EDO	B	604	4/4	0.89	0.38	31,34,38,43	0
3	EDO	C	605	4/4	0.89	0.11	54,55,55,58	0
4	SO4	C	603	5/5	0.90	0.19	106,106,108,110	0
3	EDO	A	603	4/4	0.91	0.10	33,37,40,43	0
2	BEN	B	601	9/9	0.95	0.07	17,22,25,26	0
2	BEN	C	601	9/9	0.95	0.07	18,19,22,22	0
3	EDO	C	606	4/4	0.96	0.12	45,54,57,59	0
2	BEN	A	601	9/9	0.96	0.07	14,16,19,19	0

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

There are no such residues in this entry.