



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N2X  
Title : Crystal structure of YagE, a prophage protein belonging to the dihydrodipicolinic acid synthase family from E. coli K12 in complex with pyruvate  
Authors : Bhaskar, V.; Kumar, P.M.; Manicka, S.; Krishnaswamy, S.  
Deposited on : 2010-05-19  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

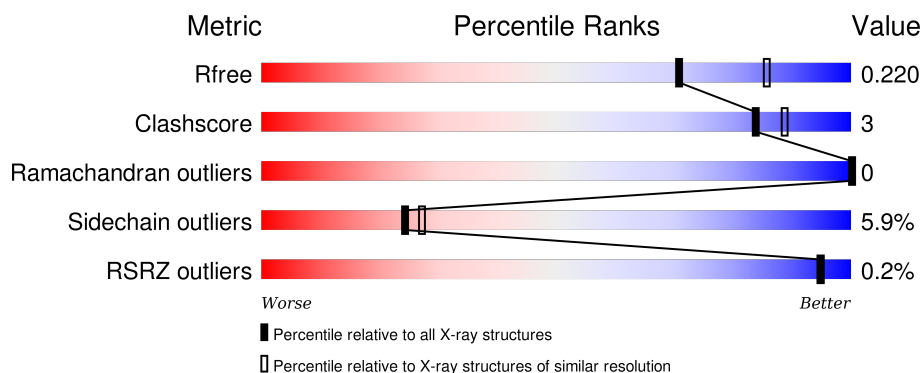
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	298	<div> <div>90%</div> <div>8% ..</div> </div>
1	B	298	<div> <div>92%</div> <div>5% ..</div> </div>
1	C	298	<div> <div>86%</div> <div>12% ..</div> </div>
1	D	298	<div> <div>88%</div> <div>9% ..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MCL	A	174	X	-	-	-
1	MCL	B	174	X	-	-	-
1	MCL	C	174	X	-	-	-
1	MCL	D	174	X	-	-	-
2	EDO	A	1	-	-	-	X
2	EDO	B	2	-	-	-	X
2	EDO	C	3	-	-	-	X
2	EDO	D	4	-	-	-	X

## 2 Entry composition [i](#)

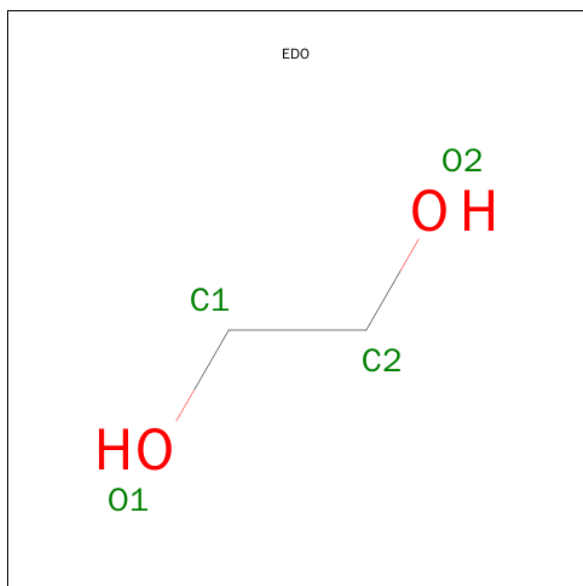
There are 3 unique types of molecules in this entry. The entry contains 9576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein yagE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2263	1449	385	423	6			
1	B	298	Total	C	N	O	S	0	0	0
			2265	1450	388	421	6			
1	C	298	Total	C	N	O	S	0	1	0
			2269	1454	388	421	6			
1	D	298	Total	C	N	O	S	0	0	0
			2268	1451	388	423	6			

- Molecule 2 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
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	136	Total	O	0	0
			136	136		
3	C	117	Total	O	0	0
			117	117		
3	D	119	Total	O	0	0
			119	119		

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Uncharacterized protein yagE

Chain A:  90% 8% ..




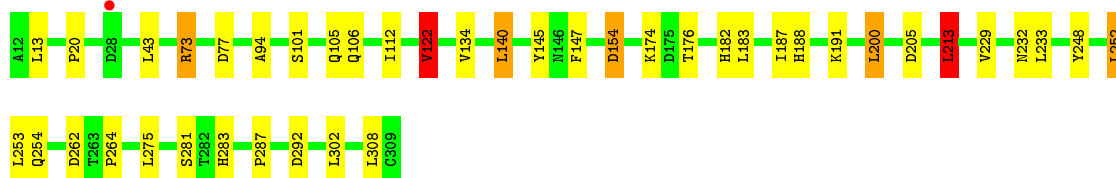
- Molecule 1: Uncharacterized protein yagE

Chain B:  92% 5% ..




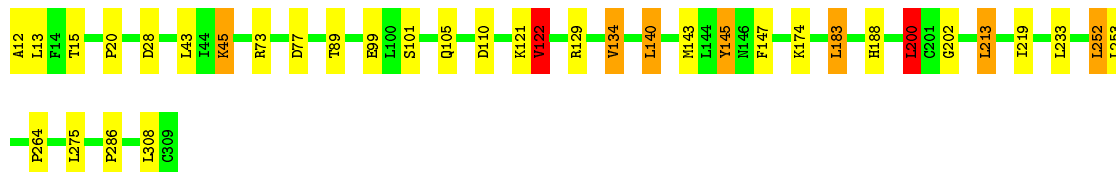
- Molecule 1: Uncharacterized protein yagE

Chain C:  86% 12% ..



- Molecule 1: Uncharacterized protein yagE

Chain D:  88% 9% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.13Å 153.55Å 55.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.20 48.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.98-2.20) 99.3 (48.98-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.37 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.179 , 0.222 0.177 , 0.220	Depositor DCC
$R_{free}$ test set	3097 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.4	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 62107 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.91 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2019e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: MCL, 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	1.03	0/2296	1.00	9/3129 (0.3%)
1	B	0.96	0/2298	0.91	8/3131 (0.3%)
1	C	1.00	2/2303 (0.1%)	1.04	10/3138 (0.3%)
1	D	1.10	4/2301 (0.2%)	0.98	16/3135 (0.5%)
All	All	1.02	6/9198 (0.1%)	0.98	43/12533 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	1	0
1	C	1	0
1	D	1	0
All	All	4	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	134	VAL	CB-CG2	-12.41	1.26	1.52
1	D	15	THR	CB-OG1	-12.06	1.19	1.43
1	D	134	VAL	CB-CG1	-11.99	1.27	1.52
1	D	99	GLU	CG-CD	5.44	1.60	1.51
1	C	106	GLN	CD-NE2	-5.42	1.19	1.32
1	C	134	VAL	CB-CG2	-5.04	1.42	1.52

All (43) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	ARG	NE-CZ-NH1	-19.66	110.47	120.30
1	A	73	ARG	NE-CZ-NH1	-19.13	110.73	120.30
1	C	73	ARG	NE-CZ-NH2	13.94	127.27	120.30
1	D	77	ASP	CB-CG-OD1	12.33	129.40	118.30
1	A	73	ARG	NE-CZ-NH2	12.14	126.37	120.30
1	A	77	ASP	CB-CG-OD1	8.87	126.28	118.30
1	A	45	LYS	CD-CE-NZ	-8.52	92.10	111.70
1	C	77	ASP	CB-CG-OD1	8.43	125.89	118.30
1	D	134	VAL	CG1-CB-CG2	-8.40	97.46	110.90
1	C	122	VAL	CG1-CB-CG2	7.56	123.00	110.90
1	B	122	VAL	CG1-CB-CG2	7.47	122.86	110.90
1	A	292	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	122	VAL	CG1-CB-CG2	7.24	122.49	110.90
1	D	15	THR	CA-CB-OG1	6.97	123.64	109.00
1	C	292	ASP	CB-CG-OD1	6.96	124.56	118.30
1	D	77	ASP	OD1-CG-OD2	-6.85	110.29	123.30
1	D	73	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	B	77	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	213	LEU	CB-CG-CD1	6.49	122.04	111.00
1	B	252	LEU	CB-CG-CD1	6.44	121.94	111.00
1	A	122	VAL	CG1-CB-CG2	6.01	120.51	110.90
1	D	110	ASP	CB-CG-OD2	5.91	123.62	118.30
1	C	213	LEU	CB-CG-CD1	5.78	120.83	111.00
1	B	213	LEU	CB-CG-CD1	5.72	120.72	111.00
1	B	45	LYS	CD-CE-NZ	-5.71	98.58	111.70
1	A	252	LEU	CB-CG-CD1	5.65	120.61	111.00
1	D	121	LYS	CD-CE-NZ	-5.55	98.93	111.70
1	C	154	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	200	LEU	CB-CG-CD1	5.37	120.12	111.00
1	D	45	LYS	CD-CE-NZ	-5.36	99.37	111.70
1	D	200	LEU	CB-CG-CD1	5.34	120.09	111.00
1	A	213	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	205	ASP	CB-CG-OD1	5.23	123.01	118.30
1	D	252	LEU	CB-CG-CD1	5.20	119.84	111.00
1	D	183	LEU	CB-CG-CD1	5.17	119.79	111.00
1	D	122	VAL	N-CA-CB	-5.16	100.16	111.50
1	D	45	LYS	CB-CG-CD	-5.13	98.27	111.60
1	B	183	LEU	CB-CG-CD1	5.12	119.71	111.00
1	C	213	LEU	CA-CB-CG	5.10	127.03	115.30
1	D	213	LEU	CB-CG-CD1	5.10	119.67	111.00
1	D	73	ARG	CG-CD-NE	-5.09	101.11	111.80
1	B	292	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	122	VAL	N-CA-CB	-5.02	100.45	111.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	174	MCL	CX1
1	B	174	MCL	CX1
1	C	174	MCL	CX1
1	D	174	MCL	CX1

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	2263	0	2282	18	0
1	B	2265	0	2289	8	0
1	C	2269	0	2286	24	1
1	D	2268	0	2291	18	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
2	D	4	0	6	2	0
3	A	123	0	0	5	0
3	B	136	0	0	2	1
3	C	117	0	0	4	0
3	D	119	0	0	4	0
All	All	9576	0	9172	55	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 3.

All (55) 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:174:MCL:HX1	3:D:444:HOH:O	1.61	0.98
1:A:174:MCL:HX1	3:A:354:HOH:O	1.63	0.97
1:C:174:MCL:HX1	3:C:381:HOH:O	1.73	0.87
1:D:129:ARG:HD2	3:D:374:HOH:O	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:VAL:HG22	1:D:264:PRO:HD3	1.65	0.77
1:C:264:PRO:HD3	1:D:122:VAL:HG22	1.66	0.77
1:A:264:PRO:HD3	1:B:122:VAL:HG22	1.68	0.76
1:A:122:VAL:HG22	1:B:264:PRO:HD3	1.70	0.74
1:C:281:SER:OG	1:C:283[B]:HIS:HD2	1.72	0.72
1:A:209:ASN:ND2	3:A:489:HOH:O	2.23	0.70
1:B:188:HIS:CE1	3:B:362:HOH:O	2.45	0.70
1:D:20:PRO:HG3	1:D:174:MCL:H12	1.75	0.69
1:B:105:GLN:HB2	1:B:140:LEU:HD22	1.78	0.66
1:B:174:MCL:HX1	3:B:397:HOH:O	1.94	0.66
1:C:281:SER:OG	1:C:283[B]:HIS:CD2	2.50	0.65
1:A:188:HIS:HB3	3:A:452:HOH:O	1.97	0.63
1:A:213:LEU:HD13	1:C:253:LEU:HB3	1.85	0.58
1:D:145:TYR:HD1	2:D:4:EDO:H21	1.69	0.58
1:D:188:HIS:CE1	3:D:445:HOH:O	2.57	0.57
1:A:188:HIS:CE1	3:A:475:HOH:O	2.56	0.56
1:D:105:GLN:HB2	1:D:140:LEU:HD22	1.86	0.56
1:A:28:ASP:N	1:A:28:ASP:OD1	2.37	0.55
1:A:105:GLN:HB2	1:A:140:LEU:HD22	1.89	0.54
1:D:12:ALA:N	3:D:442:HOH:O	2.41	0.53
1:C:174:MCL:O1	3:C:380:HOH:O	2.18	0.51
1:A:20:PRO:HG3	1:A:174:MCL:H12	1.93	0.51
1:A:253:LEU:HB3	1:C:213:LEU:HD13	1.92	0.50
1:A:188:HIS:HE1	1:C:254:GLN:OE1	1.93	0.50
1:D:89:THR:HG21	1:D:101:SER:HA	1.94	0.49
1:D:145:TYR:CD1	2:D:4:EDO:H21	2.48	0.49
1:C:176:THR:HG21	3:C:381:HOH:O	2.14	0.48
1:C:94:ALA:HB3	1:D:286:PRO:HB2	1.96	0.47
1:A:232:ASN:HB3	1:A:248:TYR:CZ	2.49	0.47
1:A:233:LEU:HD23	1:A:233:LEU:C	2.35	0.47
1:D:143:MET:HE2	1:D:200:LEU:HD22	1.97	0.46
1:B:20:PRO:HG3	1:B:174:MCL:H12	1.96	0.46
1:C:20:PRO:HG3	1:C:174:MCL:H12	1.98	0.45
1:D:143:MET:CE	1:D:200:LEU:HD22	2.47	0.45
1:A:254:GLN:OE1	1:C:188:HIS:CE1	2.70	0.45
1:D:233:LEU:HD23	1:D:233:LEU:C	2.37	0.45
1:C:262:ASP:OD1	3:C:485:HOH:O	2.21	0.45
1:B:17:ILE:HD12	1:B:230:SER:HB3	1.99	0.45
1:C:229:VAL:HG11	1:C:252:LEU:HD13	2.00	0.44
1:C:105:GLN:HB2	1:C:140:LEU:HD22	2.00	0.44
1:A:176:THR:HG21	3:A:354:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LEU:C	1:C:233:LEU:HD23	2.39	0.42
1:C:232:ASN:HB3	1:C:248:TYR:CZ	2.55	0.42
1:D:202:GLY:HA2	1:D:219:ILE:O	2.19	0.42
1:A:188:HIS:CE1	1:C:254:GLN:OE1	2.72	0.42
1:A:254:GLN:OE1	1:C:188:HIS:HE1	2.02	0.41
1:C:287:PRO:HG2	1:D:122:VAL:HG21	2.01	0.41
1:B:213:LEU:HD13	1:D:253:LEU:HB3	2.03	0.41
1:C:154:ASP:OD2	1:C:182:HIS:NE2	2.54	0.41
1:C:187:ILE:O	1:C:191:LYS:HB2	2.20	0.41
1:C:101:SER:HB3	1:C:112:ILE:HD13	2.04	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)
1:C:73:ARG:NH2	3:B:430:HOH:O[4_454]	2.18	0.02

## 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	295/298 (99%)	288 (98%)	7 (2%)	0	100	100
1	B	295/298 (99%)	290 (98%)	5 (2%)	0	100	100
1	C	296/298 (99%)	291 (98%)	5 (2%)	0	100	100
1	D	295/298 (99%)	289 (98%)	6 (2%)	0	100	100
All	All	1181/1192 (99%)	1158 (98%)	23 (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	A	241/242 (100%)	227 (94%)	14 (6%)	25	28
1	B	241/242 (100%)	226 (94%)	15 (6%)	23	25
1	C	240/242 (99%)	227 (95%)	13 (5%)	27	31
1	D	242/242 (100%)	227 (94%)	15 (6%)	23	25
All	All	964/968 (100%)	907 (94%)	57 (6%)	24	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	28	ASP
1	A	43	LEU
1	A	45	LYS
1	A	122	VAL
1	A	140	LEU
1	A	145	TYR
1	A	147	PHE
1	A	183	LEU
1	A	200	LEU
1	A	213	LEU
1	A	252	LEU
1	A	275	LEU
1	A	308	LEU
1	B	13	LEU
1	B	28	ASP
1	B	43	LEU
1	B	45	LYS
1	B	122	VAL
1	B	140	LEU
1	B	145	TYR
1	B	147	PHE
1	B	183	LEU
1	B	188	HIS

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Mol	Chain	Res	Type
1	B	200	LEU
1	B	213	LEU
1	B	252	LEU
1	B	275	LEU
1	B	308	LEU
1	C	13	LEU
1	C	43	LEU
1	C	122	VAL
1	C	140	LEU
1	C	145	TYR
1	C	147	PHE
1	C	183	LEU
1	C	200	LEU
1	C	213	LEU
1	C	252	LEU
1	C	275	LEU
1	C	302	LEU
1	C	308	LEU
1	D	13	LEU
1	D	28	ASP
1	D	43	LEU
1	D	45	LYS
1	D	122	VAL
1	D	134	VAL
1	D	140	LEU
1	D	145	TYR
1	D	147	PHE
1	D	183	LEU
1	D	200	LEU
1	D	213	LEU
1	D	252	LEU
1	D	275	LEU
1	D	308	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	102	GLN
1	A	106	GLN
1	A	188	HIS
1	A	254	GLN

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Mol	Chain	Res	Type
1	A	257	GLN
1	B	62	GLN
1	B	102	GLN
1	B	254	GLN
1	B	257	GLN
1	C	62	GLN
1	C	102	GLN
1	C	188	HIS
1	D	62	GLN
1	D	102	GLN
1	D	188	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	MCL	A	174	1	10,13,14	3.48	1 (10%)	9,15,17	1.90	3 (33%)
1	MCL	B	174	1	10,13,14	3.04	2 (20%)	9,15,17	1.44	2 (22%)
1	MCL	C	174	1	10,13,14	3.16	1 (10%)	9,15,17	1.92	2 (22%)
1	MCL	D	174	1	10,13,14	3.43	1 (10%)	9,15,17	1.90	2 (22%)

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	MCL	A	174	1	1/1/3/4	0/8/14/16	0/0/0/0
1	MCL	B	174	1	1/1/3/4	0/8/14/16	0/0/0/0
1	MCL	C	174	1	1/1/3/4	0/8/14/16	0/0/0/0
1	MCL	D	174	1	1/1/3/4	0/8/14/16	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	MCL	CE-NZ	-2.34	1.41	1.47
1	B	174	MCL	CX1-NZ	8.78	1.43	1.29
1	C	174	MCL	CX1-NZ	9.68	1.44	1.29
1	D	174	MCL	CX1-NZ	10.62	1.46	1.29
1	A	174	MCL	CX1-NZ	10.67	1.46	1.29

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	174	MCL	O-C-CA	-4.17	114.63	125.49
1	C	174	MCL	O-C-CA	-3.35	116.77	125.49
1	A	174	MCL	O-C-CA	-3.12	117.36	125.49
1	C	174	MCL	C1-CX1-NZ	-3.09	115.21	123.14
1	A	174	MCL	C1-CX1-NZ	-2.86	115.80	123.14
1	D	174	MCL	C1-CX1-CX2	-2.74	111.04	119.11
1	A	174	MCL	C1-CX1-CX2	-2.58	111.52	119.11
1	B	174	MCL	O-C-CA	-2.41	119.22	125.49
1	B	174	MCL	C1-CX1-NZ	-2.02	117.97	123.14

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	174	MCL	CX1
1	C	174	MCL	CX1
1	B	174	MCL	CX1
1	D	174	MCL	CX1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	174	MCL	2	0
1	B	174	MCL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	174	MCL	3	0
1	D	174	MCL	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	EDO	A	1	-	3,3,3	0.38	0	2,2,2	0.76	0
2	EDO	B	2	-	3,3,3	0.33	0	2,2,2	2.01	1 (50%)
2	EDO	C	3	-	3,3,3	0.61	0	2,2,2	0.73	0
2	EDO	D	4	-	3,3,3	0.49	0	2,2,2	0.64	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	A	1	-	-	0/1/1/1	0/0/0/0
2	EDO	B	2	-	-	0/1/1/1	0/0/0/0
2	EDO	C	3	-	-	0/1/1/1	0/0/0/0
2	EDO	D	4	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	2	EDO	O2-C2-C1	-2.61	93.81	112.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	EDO	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

### 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	A	297/298 (99%)	-0.56	1 (0%) 94 94	7, 12, 23, 35	0
1	B	297/298 (99%)	-0.54	0 100 100	7, 12, 22, 34	0
1	C	297/298 (99%)	-0.67	1 (0%) 94 94	7, 12, 23, 33	0
1	D	297/298 (99%)	-0.68	0 100 100	7, 12, 23, 34	0
All	All	1188/1192 (99%)	-0.61	2 (0%) 95 95	7, 12, 23, 35	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	ASP	2.2
1	A	302	LEU	2.1

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	MCL	A	174	14/15	0.97	0.10	-	5,9,19,22	0
1	MCL	C	174	14/15	0.97	0.12	-	6,9,19,23	0
1	MCL	B	174	14/15	0.96	0.12	-	6,9,19,22	0
1	MCL	D	174	14/15	0.95	0.09	-	5,9,19,23	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	C	3	4/4	0.95	0.15	7.01	17,17,18,24	0
2	EDO	D	4	4/4	0.96	0.14	4.17	9,18,22,26	0
2	EDO	B	2	4/4	0.96	0.15	3.25	13,14,17,20	0
2	EDO	A	1	4/4	0.96	0.12	2.41	16,20,20,26	0

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

There are no such residues in this entry.