



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:35 pm GMT

PDB ID : 2FEF  
Title : The Crystal Structure of Protein PA2201 from *Pseudomonas aeruginosa*  
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Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2005-12-15  
Resolution : 1.90 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

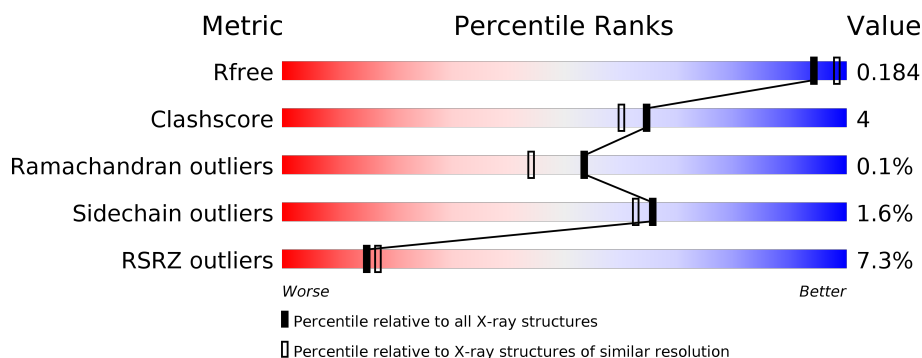
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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	294	<div> <div>9%</div> <div>88%</div> <div>7% . .</div> </div>
1	B	294	<div> <div>4%</div> <div>90%</div> <div>5% . .</div> </div>
1	C	294	<div> <div>7%</div> <div>89%</div> <div>6% . .</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
2	EDO	C	603	-	-	X	-

## 2 Entry composition [i](#)

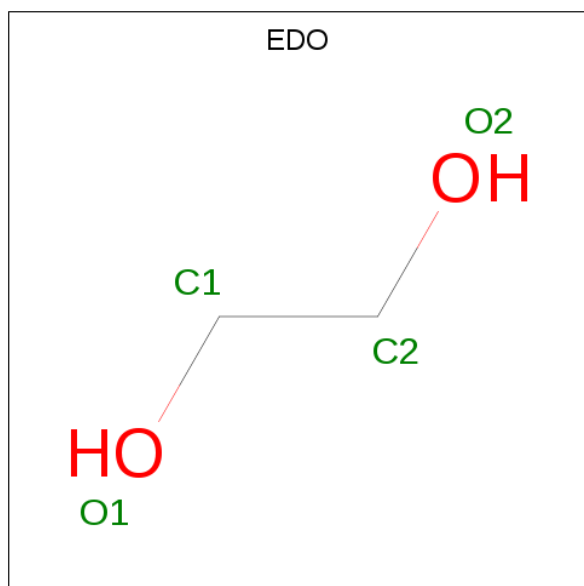
There are 3 unique types of molecules in this entry. The entry contains 7187 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 hypothetical protein PA2201.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	Se	0	4	1
			2217	1424	394	397	2			
1	B	284	Total	C	N	O	Se	0	5	0
			2255	1444	405	404	2			
1	C	281	Total	C	N	O	Se	0	5	1
			2223	1427	396	398	2			

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

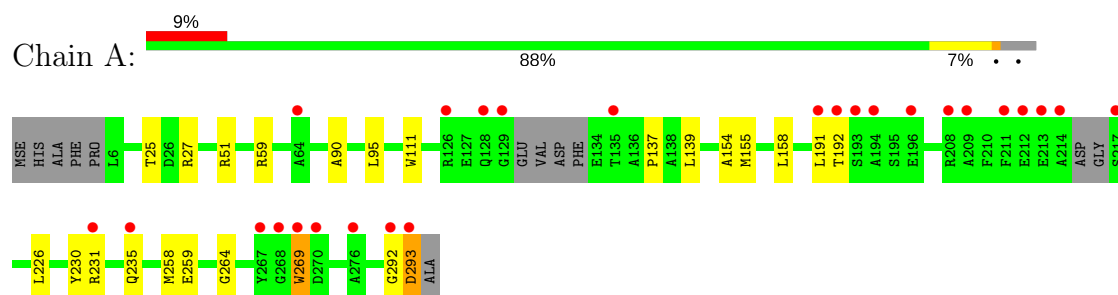
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	162	Total	O	0	0
			162	162		
3	C	172	Total	O	0	0
			172	172		

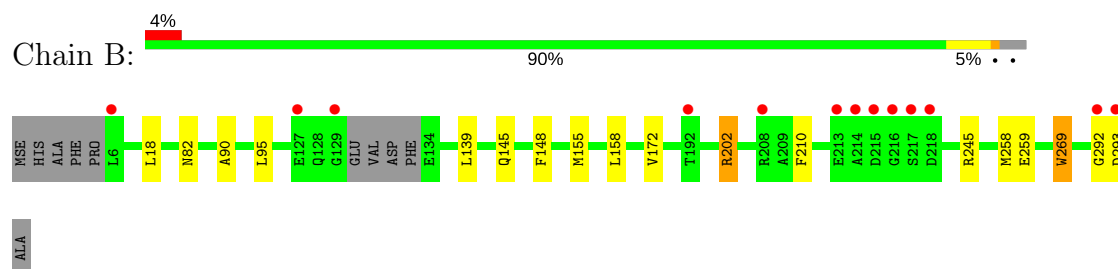
### 3 Residue-property plots [i](#)

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

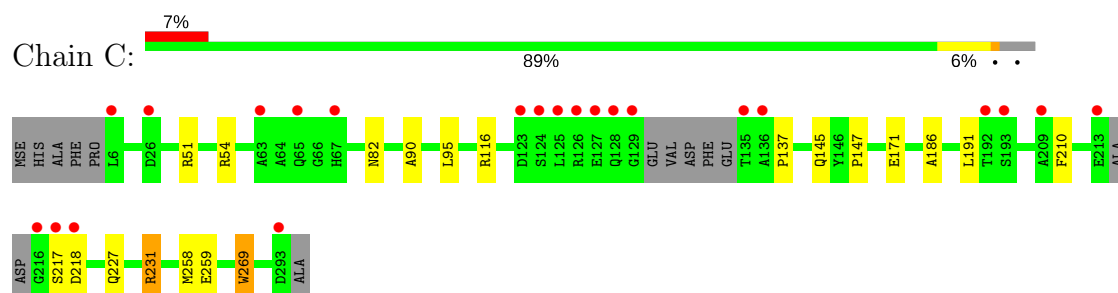
#### • Molecule 1: hypothetical protein PA2201



#### • Molecule 1: hypothetical protein PA2201



#### • Molecule 1: hypothetical protein PA2201



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.59Å 118.59Å 144.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.83 – 1.90 45.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.83-1.90) 98.8 (45.81-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.186 , 0.222 0.188 , 0.184	Depositor DCC
$R_{free}$ test set	4070 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: 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	0.66	0/2283	0.70	1/3101 (0.0%)
1	B	0.70	0/2322	0.70	0/3155
1	C	0.76	0/2293	0.73	1/3116 (0.0%)
All	All	0.71	0/6898	0.71	2/9372 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	258	MSE	CG-SE-CE	-5.84	86.06	98.90
1	A	59	ARG	NE-CZ-NH2	-5.40	117.60	120.30

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	2217	0	2141	18	0
1	B	2255	0	2195	21	0
1	C	2223	0	2158	22	0
2	B	8	0	12	0	0
2	C	8	0	12	4	0
3	A	142	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	162	0	0	0	0
3	C	172	0	0	4	0
All	All	7187	0	6518	59	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 4.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:PRO:HB2	2:C:603:EDO:H12	1.22	1.16
1:A:155:MSE:HE1	1:A:158:LEU:HD12	1.41	1.02
1:A:155:MSE:CE	1:A:158:LEU:HD12	1.92	0.98
1:A:51[B]:ARG:HH12	1:C:82:ASN:HD21	1.24	0.84
1:A:155:MSE:HE1	1:A:158:LEU:CD1	2.08	0.84
1:C:147:PRO:HB2	2:C:603:EDO:C1	2.10	0.76
1:B:155:MSE:HE3	1:B:258:MSE:SE	2.40	0.72
1:C:147:PRO:CB	2:C:603:EDO:H12	2.12	0.72
1:B:82:ASN:HD21	1:C:51[B]:ARG:HH12	1.37	0.70
1:A:292:GLY:O	1:A:293:ASP:HB2	1.91	0.69
1:C:210:PHE:CE1	1:C:269[A]:TRP:CH2	2.81	0.69
1:C:210:PHE:HE1	1:C:269[A]:TRP:CZ3	2.11	0.69
1:A:155:MSE:HE2	1:A:158:LEU:HD12	1.75	0.67
1:B:245:ARG:HG2	1:B:245:ARG:HH11	1.60	0.67
1:B:155:MSE:CE	1:B:158:LEU:HD12	2.27	0.65
1:A:231:ARG:O	1:A:235:GLN:HG3	1.98	0.64
1:B:155:MSE:HE3	1:B:258:MSE:CG	2.27	0.64
1:A:137:PRO:HG3	3:A:304:HOH:O	2.00	0.62
1:C:116:ARG:NH2	1:C:171:GLU:OE1	2.22	0.62
1:C:210:PHE:CE1	1:C:269[A]:TRP:CZ3	2.88	0.61
1:A:137:PRO:CG	3:A:304:HOH:O	2.48	0.61
1:B:155:MSE:HE1	1:B:158:LEU:HD12	1.81	0.60
1:C:137:PRO:HG3	3:C:610:HOH:O	2.01	0.60
1:A:90:ALA:HB1	1:A:95:LEU:HD12	1.86	0.57
1:B:202:ARG:HG2	1:B:245:ARG:HG3	1.87	0.57
1:C:210:PHE:CE1	1:C:269[A]:TRP:HH2	2.27	0.53
1:B:18:LEU:HD12	1:B:18:LEU:N	2.25	0.52
1:C:90:ALA:HB1	1:C:95:LEU:HD12	1.90	0.52
1:A:264:GLY:HA2	1:A:269:TRP:CZ3	2.48	0.49
1:C:186:ALA:HA	1:C:191:LEU:HB2	1.95	0.49
1:C:116:ARG:NE	1:C:171:GLU:OE2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145[B]:GLN:HE22	1:C:54:ARG:HH22	1.62	0.48
1:A:226:LEU:O	1:A:230:TYR:HB2	2.14	0.48
1:C:210:PHE:HE1	1:C:269[A]:TRP:CH2	2.27	0.48
1:B:155:MSE:HE3	1:B:258:MSE:HB3	1.95	0.47
1:C:210:PHE:CZ	1:C:269[A]:TRP:HH2	2.33	0.47
1:B:155:MSE:HE1	1:B:158:LEU:CD1	2.46	0.46
1:B:90:ALA:HB1	1:B:95:LEU:HD12	1.96	0.46
1:C:210:PHE:CZ	1:C:269[A]:TRP:CH2	3.04	0.45
2:C:603:EDO:C2	3:C:729:HOH:O	2.65	0.45
1:A:25:THR:OG1	1:A:27:ARG:HG2	2.17	0.45
1:B:292:GLY:O	1:B:293:ASP:HB2	2.16	0.44
1:A:155:MSE:CE	1:A:258:MSE:HG2	2.48	0.44
1:C:227:GLN:OE1	1:C:231[B]:ARG:HD3	2.18	0.43
1:B:18:LEU:HD12	1:B:18:LEU:H	1.82	0.43
1:B:245:ARG:NH1	1:B:245:ARG:HG2	2.30	0.43
1:A:111:TRP:CZ3	1:A:139:LEU:HD13	2.54	0.43
1:C:218:ASP:HA	3:C:684:HOH:O	2.19	0.43
1:B:155:MSE:CE	1:B:258:MSE:HG2	2.49	0.43
1:B:210:PHE:HE1	1:B:269:TRP:CZ3	2.35	0.43
1:B:139[A]:LEU:HD11	1:B:148:PHE:HB2	2.01	0.42
1:C:217:SER:HB3	1:C:218:ASP:H	1.65	0.42
1:A:111:TRP:CH2	1:A:139:LEU:HD13	2.55	0.42
1:B:155:MSE:HE3	1:B:258:MSE:CB	2.49	0.42
1:A:154:ALA:C	1:A:155:MSE:HE2	2.41	0.42
1:B:155:MSE:CE	1:B:258:MSE:HB3	2.50	0.42
1:C:145:GLN:HG2	3:C:761:HOH:O	2.20	0.41
1:A:137:PRO:HG2	3:A:304:HOH:O	2.18	0.40
1:B:139[B]:LEU:HB2	1:B:172:VAL:HG12	2.02	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	280/294 (95%)	271 (97%)	8 (3%)	1 (0%)	36	25
1	B	285/294 (97%)	279 (98%)	6 (2%)	0	100	100
1	C	280/294 (95%)	270 (96%)	10 (4%)	0	100	100
All	All	845/882 (96%)	820 (97%)	24 (3%)	1 (0%)	53	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	THR

### 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	207/222 (93%)	203 (98%)	4 (2%)	60	55
1	B	213/222 (96%)	210 (99%)	3 (1%)	69	67
1	C	210/222 (95%)	205 (98%)	5 (2%)	52	45
All	All	630/666 (95%)	618 (98%)	12 (2%)	65	55

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	A	259	GLU
1	A	269	TRP
1	A	293	ASP
1	B	202	ARG
1	B	259	GLU
1	B	269	TRP
1	C	231[A]	ARG
1	C	231[B]	ARG
1	C	259	GLU
1	C	269[A]	TRP
1	C	269[B]	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
1	C	82	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	B	601	-	3,3,3	0.57	0	2,2,2	0.31	0
2	EDO	B	604	-	3,3,3	0.43	0	2,2,2	0.65	0
2	EDO	C	602	-	3,3,3	0.40	0	2,2,2	0.69	0
2	EDO	C	603	-	3,3,3	0.20	0	2,2,2	2.50	2 (100%)

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	B	601	-	-	0/1/1/1	0/0/0/0
2	EDO	B	604	-	-	0/1/1/1	0/0/0/0
2	EDO	C	602	-	-	0/1/1/1	0/0/0/0
2	EDO	C	603	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	603	EDO	O1-C1-C2	-2.51	94.40	112.09
2	C	603	EDO	O2-C2-C1	-2.49	94.48	112.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	603	EDO	4	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	280/294 (95%)	0.54	26 (9%) 8 10	19, 28, 44, 55	0
1	B	282/294 (95%)	0.42	13 (4%) 32 36	23, 28, 42, 52	0
1	C	279/294 (94%)	0.54	22 (7%) 12 14	22, 27, 44, 53	0
All	All	841/882 (95%)	0.50	61 (7%) 15 17	19, 28, 44, 55	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	ALA	8.1
1	A	193	SER	5.7
1	C	216	GLY	4.7
1	A	191	LEU	4.5
1	B	293	ASP	4.5
1	C	128	GLN	4.3
1	B	214	ALA	4.3
1	C	209	ALA	4.2
1	C	127	GLU	4.0
1	A	194	ALA	4.0
1	C	124	SER	3.8
1	A	209	ALA	3.8
1	A	293	ASP	3.8
1	B	216	GLY	3.7
1	B	217	SER	3.7
1	C	135	THR	3.5
1	A	135	THR	3.5
1	C	192	THR	3.5
1	A	208	ARG	3.4
1	C	193	SER	3.4
1	A	217	SER	3.3
1	C	26	ASP	3.3
1	A	292	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	63	ALA	3.2
1	B	215	ASP	3.1
1	C	293	ASP	2.9
1	B	6	LEU	2.9
1	A	126	ARG	2.9
1	A	192	THR	2.9
1	C	67	HIS	2.8
1	A	129	GLY	2.8
1	A	64	ALA	2.7
1	A	270	ASP	2.7
1	B	127	GLU	2.7
1	A	128	GLN	2.6
1	C	218	ASP	2.6
1	A	276	ALA	2.6
1	A	211	PHE	2.6
1	A	213	GLU	2.5
1	B	129	GLY	2.5
1	B	292	GLY	2.5
1	B	208	ARG	2.5
1	C	126	ARG	2.4
1	C	125	LEU	2.4
1	C	129	GLY	2.4
1	A	268	GLY	2.3
1	C	65	GLN	2.3
1	B	213	GLU	2.3
1	C	123	ASP	2.3
1	C	136	ALA	2.3
1	B	218	ASP	2.3
1	A	235	GLN	2.2
1	A	269	TRP	2.2
1	A	267	TYR	2.2
1	C	6	LEU	2.1
1	C	217	SER	2.1
1	A	212	GLU	2.1
1	A	196	GLU	2.1
1	B	192	THR	2.1
1	A	231	ARG	2.0
1	C	213	GLU	2.0

## 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	C	602	4/4	0.84	0.16	58,59,60,61	0
2	EDO	B	604	4/4	0.87	0.17	57,57,58,59	0
2	EDO	B	601	4/4	0.95	0.16	32,35,38,45	0
2	EDO	C	603	4/4	0.97	0.17	28,31,32,37	0

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

There are no such residues in this entry.