



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2017 – 05:01 PM EST

PDB ID : 5KDW  
Title : IMPa metallopeptidase from *Pseudomonas aeruginosa*  
Authors : Noach, I.; Boraston, A.B.  
Deposited on : 2016-06-08  
Resolution : 1.85 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

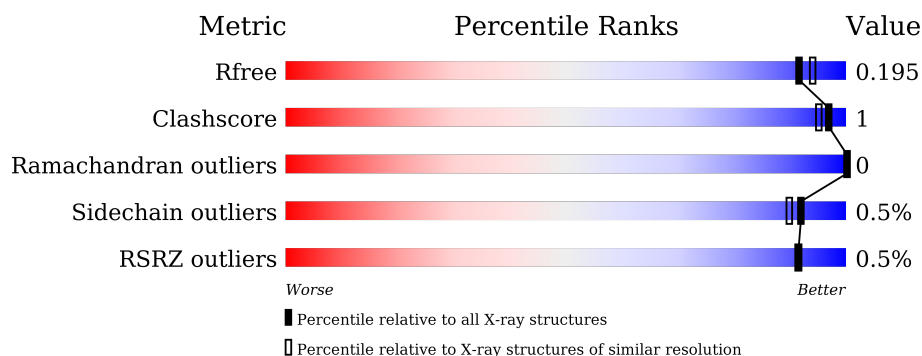
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	885	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 95%; height: 10px; background-color: green;"></div> <div style="width: 95%; text-align: center;">95%</div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; text-align: center;">.</div> </div>
1	B	885	<div> <div style="width: 96%; height: 10px; background-color: green;"></div> <div style="width: 96%; text-align: center;">96%</div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; text-align: center;">.</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	A	1005	-	-	-	X
2	EDO	A	1007	-	-	-	X
2	EDO	A	1008	-	-	-	X
2	EDO	A	1010	-	-	-	X
2	EDO	A	1011	-	-	-	X
2	EDO	A	1012	-	-	-	X
2	EDO	A	1015	-	-	-	X
2	EDO	A	1016	-	-	-	X
2	EDO	A	1017	-	-	-	X
2	EDO	A	1018	-	-	-	X
2	EDO	A	1019	-	-	-	X
2	EDO	A	1021	-	-	-	X
2	EDO	B	1001	-	-	-	X
2	EDO	B	1004	-	-	-	X
2	EDO	B	1006	-	-	-	X
2	EDO	B	1008	-	-	-	X
2	EDO	B	1009	-	-	-	X
2	EDO	B	1011	-	-	-	X
2	EDO	B	1013	-	-	-	X
2	EDO	B	1016	-	-	-	X
2	EDO	B	1018	-	-	-	X
2	EDO	B	1021	-	-	-	X
4	PO4	A	1023	-	-	-	X
4	PO4	A	1024	-	-	X	-
4	PO4	A	1025	-	-	X	X
4	PO4	A	1026	-	-	-	X
4	PO4	B	1023	-	-	-	X
4	PO4	B	1025	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15932 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.

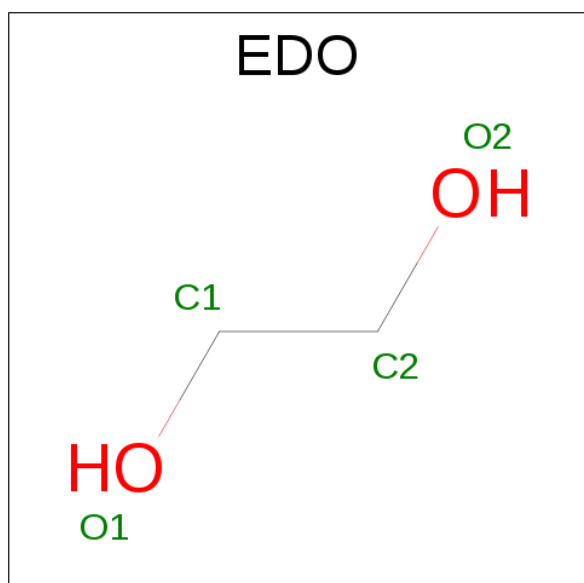
- Molecule 1 is a protein called Metallopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	883	Total	C	N	O	S	0	9	0
			6843	4278	1225	1324	16			
1	B	883	Total	C	N	O	S	0	8	0
			6824	4268	1220	1320	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	initiating methionine	UNP Q9I5W4
A	924	LEU	-	expression tag	UNP Q9I5W4
A	925	GLU	-	expression tag	UNP Q9I5W4
B	41	MET	-	initiating methionine	UNP Q9I5W4
B	924	LEU	-	expression tag	UNP Q9I5W4
B	925	GLU	-	expression tag	UNP Q9I5W4

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

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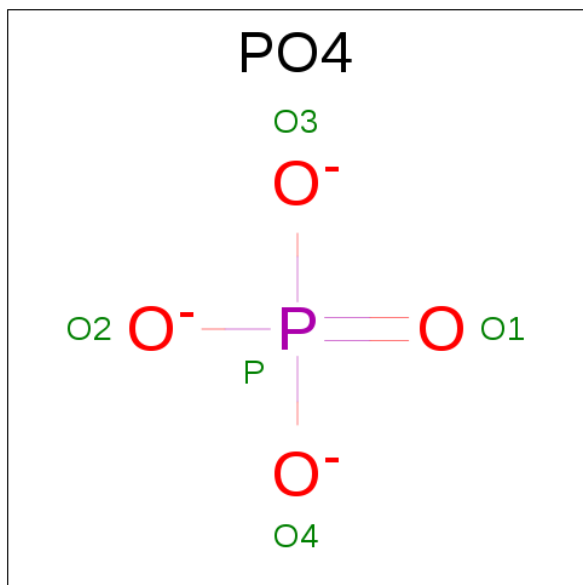
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1027	Total	O	0	0
			1027	1027		

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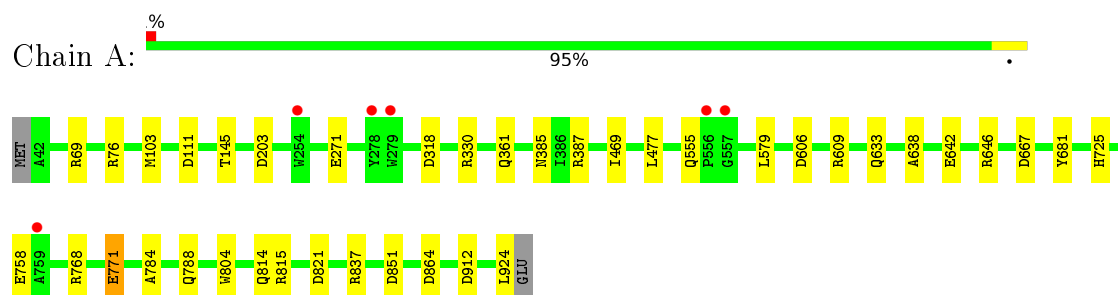
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1033	Total 1033	O 1033	0	0



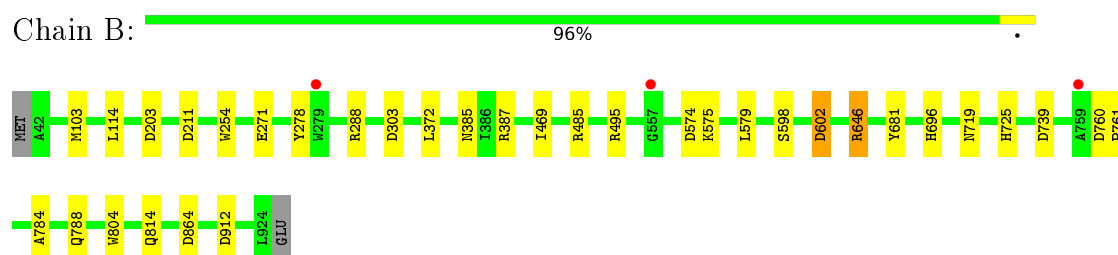
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Metallopeptidase



#### • Molecule 1: Metallopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.92Å 132.73Å 103.07Å 90.00° 103.81° 90.00°	Depositor
Resolution (Å)	100.09 – 1.85 48.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (100.09-1.85) 100.0 (48.00-1.85)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.153 , 0.186 0.165 , 0.195	Depositor DCC
$R_{free}$ test set	10928 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.065 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15932	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: ZN, PO4, 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	0.77	0/6991	0.85	17/9514 (0.2%)
1	B	0.78	0/6972	0.84	16/9490 (0.2%)
All	All	0.78	0/13963	0.85	33/19004 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	864	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	667	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	69	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	837	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	A	912	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	912	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	B	485	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	76	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	A	815	ARG	NE-CZ-NH2	6.35	123.48	120.30
1	B	303	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	646	ARG	NE-CZ-NH1	-6.05	117.27	120.30
1	B	602	ASP	CB-CA-C	-5.82	98.76	110.40
1	A	606	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	646	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	A	203	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	B	760	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	912	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	69	ARG	CG-CD-NE	-5.48	100.29	111.80
1	B	288	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	864	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	318	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	387	ARG	NE-CZ-NH1	-5.29	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	485	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	681	TYR	CA-CB-CG	5.25	123.37	113.40
1	B	387	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	851	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	821	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	609	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	681	TYR	CA-CB-CG	5.13	123.14	113.40
1	B	203	ASP	CB-CG-OD1	5.11	122.89	118.30
1	B	288	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	211	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	495	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6843	0	6626	19	0
1	B	6824	0	6604	13	0
2	A	84	0	126	2	0
2	B	84	0	126	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	20	0	0	4	0
4	B	15	0	0	0	0
5	A	1027	0	0	9	0
5	B	1033	0	0	3	0
All	All	15932	0	13482	36	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 1.

All (36) 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:642[A]:GLU:OE1	5:A:1102:HOH:O	1.96	0.84
1:A:771[A]:GLU:OE1	5:A:1101:HOH:O	1.96	0.83
1:A:555:GLN:HA	1:A:555:GLN:OE1	1.87	0.74
1:A:633:GLN:NE2	5:A:1104:HOH:O	2.18	0.71
1:A:646:ARG:NH1	5:A:1109:HOH:O	2.25	0.68
1:A:145:THR:OG1	5:A:1103:HOH:O	2.15	0.64
1:A:758:GLU:OE2	1:A:768[A]:ARG:NH1	2.26	0.62
1:A:638:ALA:O	1:A:642[B]:GLU:HG2	2.01	0.60
1:A:385:ASN:HB2	5:A:1679:HOH:O	2.02	0.58
1:A:103:MET:HE2	1:A:271:GLU:HG2	1.86	0.56
4:A:1024:PO4:O3	4:A:1025:PO4:O1	2.24	0.56
1:A:642[B]:GLU:O	1:A:646:ARG:HG3	2.07	0.54
1:B:103:MET:HE2	1:B:271:GLU:HG2	1.89	0.54
1:A:469:ILE:HD13	1:A:477:LEU:HD12	1.89	0.54
1:B:385:ASN:OD1	5:B:1101:HOH:O	2.19	0.51
1:A:361:GLN:HE22	2:A:1007:EDO:HO1	1.60	0.47
1:B:579:LEU:HD12	1:B:579:LEU:C	2.35	0.47
1:B:469:ILE:HD12	1:B:469:ILE:O	2.15	0.47
1:B:574:ASP:HA	5:B:1165:HOH:O	2.15	0.47
4:A:1024:PO4:O4	4:A:1025:PO4:O4	2.33	0.45
1:B:254:TRP:CE3	1:B:278:TYR:HD1	2.34	0.44
1:B:575:LYS:HA	1:B:575:LYS:HD2	1.70	0.44
1:B:598:SER:O	1:B:602:ASP:HB2	2.18	0.43
1:A:111:ASP:OD2	4:A:1026:PO4:O2	2.36	0.43
1:A:725:HIS:HD2	1:A:804:TRP:CG	2.37	0.43
4:A:1024:PO4:O2	5:A:1105:HOH:O	2.21	0.43
2:A:1016:EDO:H21	5:A:1919:HOH:O	2.18	0.42
1:A:330:ARG:NH1	5:A:1125:HOH:O	2.46	0.42
1:A:579:LEU:C	1:A:579:LEU:HD12	2.40	0.42
1:A:784:ALA:O	1:A:788:GLN:HG2	2.20	0.41
1:A:642[A]:GLU:O	1:A:646:ARG:HG3	2.21	0.41
1:B:725:HIS:HD2	1:B:804:TRP:CG	2.39	0.41
1:B:761:PRO:HD2	5:B:1463:HOH:O	2.21	0.41
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.95	0.41
1:B:696:HIS:CE1	1:B:719:ASN:HD21	2.39	0.41
1:B:784:ALA:O	1:B:788:GLN:HG2	2.21	0.40

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	A	890/885 (101%)	877 (98%)	13 (2%)	0	100	100
1	B	889/885 (100%)	875 (98%)	14 (2%)	0	100	100
All	All	1779/1770 (100%)	1752 (98%)	27 (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	707/701 (101%)	703 (99%)	4 (1%)	90	87
1	B	704/701 (100%)	700 (99%)	4 (1%)	90	87
All	All	1411/1402 (101%)	1403 (99%)	8 (1%)	92	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	771[A]	GLU
1	A	771[B]	GLU
1	A	814	GLN
1	A	924	LEU
1	B	114	LEU
1	B	646	ARG
1	B	739	ASP
1	B	814	GLN

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

Mol	Chain	Res	Type
1	A	361	GLN
1	A	428	GLN

### 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 ⓘ

Of 51 ligands modelled in this entry, 2 are monoatomic - leaving 49 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	A	1001	-	3,3,3	0.40	0	2,2,2	0.59	0
2	EDO	A	1002	-	3,3,3	0.53	0	2,2,2	0.27	0
2	EDO	A	1003	-	3,3,3	0.20	0	2,2,2	1.27	0
2	EDO	A	1004	-	3,3,3	0.44	0	2,2,2	0.54	0
2	EDO	A	1005	-	3,3,3	0.52	0	2,2,2	0.70	0
2	EDO	A	1006	-	3,3,3	0.24	0	2,2,2	0.75	0
2	EDO	A	1007	-	3,3,3	0.45	0	2,2,2	0.06	0
2	EDO	A	1008	-	3,3,3	0.78	0	2,2,2	0.55	0
2	EDO	A	1009	-	3,3,3	0.46	0	2,2,2	0.25	0
2	EDO	A	1010	-	3,3,3	0.48	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	A	1011	-	3,3,3	0.46	0	2,2,2	0.63	0
2	EDO	A	1012	-	3,3,3	0.30	0	2,2,2	0.29	0
2	EDO	A	1013	-	3,3,3	0.24	0	2,2,2	1.28	0
2	EDO	A	1014	-	3,3,3	0.44	0	2,2,2	0.67	0
2	EDO	A	1015	-	3,3,3	0.44	0	2,2,2	0.48	0
2	EDO	A	1016	-	3,3,3	0.32	0	2,2,2	0.70	0
2	EDO	A	1017	-	3,3,3	0.35	0	2,2,2	1.61	1 (50%)
2	EDO	A	1018	-	3,3,3	0.56	0	2,2,2	0.21	0
2	EDO	A	1019	-	3,3,3	0.43	0	2,2,2	0.45	0
2	EDO	A	1020	-	3,3,3	0.64	0	2,2,2	0.17	0
2	EDO	A	1021	-	3,3,3	0.56	0	2,2,2	0.26	0
4	PO4	A	1023	-	4,4,4	0.31	0	6,6,6	0.35	0
4	PO4	A	1024	-	4,4,4	0.48	0	6,6,6	0.23	0
4	PO4	A	1025	-	4,4,4	0.17	0	6,6,6	0.28	0
4	PO4	A	1026	-	4,4,4	0.38	0	6,6,6	0.30	0
2	EDO	B	1001	-	3,3,3	0.30	0	2,2,2	0.68	0
2	EDO	B	1002	-	3,3,3	0.52	0	2,2,2	0.41	0
2	EDO	B	1003	-	3,3,3	0.64	0	2,2,2	0.14	0
2	EDO	B	1004	-	3,3,3	0.30	0	2,2,2	0.33	0
2	EDO	B	1005	-	3,3,3	0.53	0	2,2,2	0.82	0
2	EDO	B	1006	-	3,3,3	0.58	0	2,2,2	0.50	0
2	EDO	B	1007	-	3,3,3	0.24	0	2,2,2	0.07	0
2	EDO	B	1008	-	3,3,3	0.31	0	2,2,2	0.47	0
2	EDO	B	1009	-	3,3,3	0.40	0	2,2,2	0.51	0
2	EDO	B	1010	-	3,3,3	0.32	0	2,2,2	0.61	0
2	EDO	B	1011	-	3,3,3	0.32	0	2,2,2	0.51	0
2	EDO	B	1012	-	3,3,3	0.28	0	2,2,2	0.72	0
2	EDO	B	1013	-	3,3,3	0.37	0	2,2,2	0.55	0
2	EDO	B	1014	-	3,3,3	0.18	0	2,2,2	1.54	0
2	EDO	B	1015	-	3,3,3	0.65	0	2,2,2	0.11	0
2	EDO	B	1016	-	3,3,3	0.60	0	2,2,2	0.41	0
2	EDO	B	1017	-	3,3,3	0.34	0	2,2,2	0.83	0
2	EDO	B	1018	-	3,3,3	0.33	0	2,2,2	0.63	0
2	EDO	B	1019	-	3,3,3	0.29	0	2,2,2	1.02	0
2	EDO	B	1020	-	3,3,3	0.26	0	2,2,2	1.14	0
2	EDO	B	1021	-	3,3,3	0.65	0	2,2,2	0.18	0
4	PO4	B	1023	-	4,4,4	0.29	0	6,6,6	0.26	0
4	PO4	B	1024	-	4,4,4	0.41	0	6,6,6	0.32	0
4	PO4	B	1025	-	4,4,4	0.98	0	6,6,6	0.31	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. '-' means



no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	1001	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1002	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1003	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1004	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1005	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1006	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1007	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1008	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1009	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1010	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1011	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1012	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1013	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1014	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1015	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1016	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1017	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1018	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1019	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1020	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1021	-	-	0/1/1/1	0/0/0/0
4	PO4	A	1023	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1024	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1025	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1026	-	-	0/0/0/0	0/0/0/0
2	EDO	B	1001	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1002	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1003	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1004	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1005	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1006	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1007	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1008	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1009	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1010	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1011	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1012	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1013	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1014	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1015	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1016	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1017	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	1018	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1019	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1020	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1021	-	-	0/1/1/1	0/0/0/0
4	PO4	B	1023	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1024	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1025	-	-	0/0/0/0	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(°)	Ideal(°)
2	A	1017	EDO	O1-C1-C2	-2.12	97.74	112.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1007	EDO	1	0
2	A	1016	EDO	1	0
4	A	1024	PO4	3	0
4	A	1025	PO4	2	0
4	A	1026	PO4	1	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	883/885 (99%)	-0.64	6 (0%)	89 88	11, 20, 34, 62	0
1	B	883/885 (99%)	-0.66	3 (0%)	94 93	12, 19, 34, 55	0
All	All	1766/1770 (99%)	-0.65	9 (0%)	91 91	11, 20, 34, 62	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	557	GLY	3.7
1	A	557	GLY	3.4
1	A	278	TYR	2.8
1	A	279	TRP	2.8
1	A	759	ALA	2.7
1	B	279	TRP	2.5
1	B	759	ALA	2.4
1	A	556	PRO	2.4
1	A	254	TRP	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
2	EDO	A	1015	4/4	0.94	0.17	35.14	52,52,54,54	0
4	PO4	A	1026	5/5	0.92	0.14	15.80	30,42,43,44	0
2	EDO	A	1021	4/4	0.90	0.12	10.95	27,33,33,39	0
2	EDO	A	1016	4/4	0.87	0.12	8.05	46,47,49,55	0
4	PO4	A	1025	5/5	0.95	0.16	7.64	41,45,50,51	0
2	EDO	A	1008	4/4	0.86	0.14	7.61	34,37,41,42	0
2	EDO	A	1005	4/4	0.91	0.12	7.26	30,32,33,33	0
2	EDO	B	1013	4/4	0.87	0.18	7.26	35,40,43,44	0
2	EDO	A	1019	4/4	0.84	0.18	6.69	44,44,50,54	0
2	EDO	B	1006	4/4	0.90	0.09	5.55	26,28,29,29	0
2	EDO	B	1016	4/4	0.85	0.17	5.27	43,48,51,56	0
2	EDO	B	1021	4/4	0.82	0.17	4.75	31,33,34,38	0
2	EDO	A	1007	4/4	0.90	0.13	4.40	36,38,40,43	0
4	PO4	A	1023	5/5	0.98	0.10	4.26	25,26,32,34	0
2	EDO	B	1018	4/4	0.92	0.15	4.22	31,37,40,48	0
4	PO4	B	1025	5/5	0.95	0.11	4.08	30,30,40,41	0
2	EDO	A	1010	4/4	0.83	0.16	4.01	46,47,49,53	0
2	EDO	A	1018	4/4	0.82	0.16	3.89	33,35,36,42	0
2	EDO	A	1011	4/4	0.94	0.15	3.73	30,41,42,46	0
2	EDO	A	1017	4/4	0.94	0.15	3.18	26,34,40,55	0
2	EDO	B	1008	4/4	0.95	0.11	3.10	37,38,41,42	0
2	EDO	A	1012	4/4	0.94	0.12	3.08	34,36,37,41	0
2	EDO	B	1004	4/4	0.91	0.14	2.68	34,37,40,43	0
4	PO4	B	1023	5/5	0.95	0.14	2.59	28,35,38,39	0
2	EDO	B	1011	4/4	0.91	0.16	2.40	46,46,46,47	0
2	EDO	B	1001	4/4	0.93	0.10	2.34	23,29,29,31	0
2	EDO	B	1009	4/4	0.93	0.10	2.24	30,32,33,39	0
2	EDO	B	1019	4/4	0.94	0.10	1.82	25,30,36,44	0
2	EDO	B	1010	4/4	0.94	0.10	1.45	38,38,39,43	0
2	EDO	A	1006	4/4	0.96	0.11	1.18	31,33,34,39	0
2	EDO	B	1002	4/4	0.96	0.09	1.14	19,22,24,24	0
2	EDO	A	1009	4/4	0.94	0.08	0.90	32,32,32,34	0
2	EDO	A	1020	4/4	0.66	0.19	0.61	50,52,53,55	0
2	EDO	B	1003	4/4	0.84	0.15	0.42	41,43,45,49	0
2	EDO	B	1007	4/4	0.95	0.11	0.27	35,36,37,43	0
3	ZN	B	1022	1/1	0.98	0.07	0.11	27,27,27,27	1
2	EDO	A	1003	4/4	0.94	0.10	0.01	35,36,38,42	0
4	PO4	B	1024	5/5	0.98	0.08	-0.16	23,23,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	A	1001	4/4	0.96	0.07	-0.58	27,31,33,33	0
3	ZN	A	1022	1/1	0.97	0.06	-0.61	29,29,29,29	1
2	EDO	A	1002	4/4	0.98	0.06	-0.63	17,20,21,22	0
2	EDO	B	1017	4/4	0.94	0.21	-	43,44,44,46	0
2	EDO	B	1014	4/4	0.94	0.18	-	30,35,38,38	0
2	EDO	B	1005	4/4	0.96	0.12	-	33,33,34,35	0
2	EDO	B	1012	4/4	0.90	0.12	-	40,42,44,46	0
2	EDO	B	1020	4/4	0.93	0.16	-	44,46,48,48	0
4	PO4	A	1024	5/5	0.98	0.07	-	37,43,46,47	0
2	EDO	A	1004	4/4	0.98	0.15	-	27,27,29,31	0
2	EDO	B	1015	4/4	0.96	0.12	-	26,31,31,32	0
2	EDO	A	1013	4/4	0.92	0.20	-	30,36,38,38	0
2	EDO	A	1014	4/4	0.88	0.20	-	40,45,46,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.