



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 03:50 PM BST

PDB ID : 6QPU  
Title : Crystal structure of as isolated synthetic core domain of nitrite reductase from *Ralstonia pickettii* (residues 1-331)  
Authors : Antonyuk, S.V.; Hedison, T.M.; Eady, R.R.; Hasnain, S.S.; Scrutton, N.S.  
Deposited on : 2019-02-15  
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

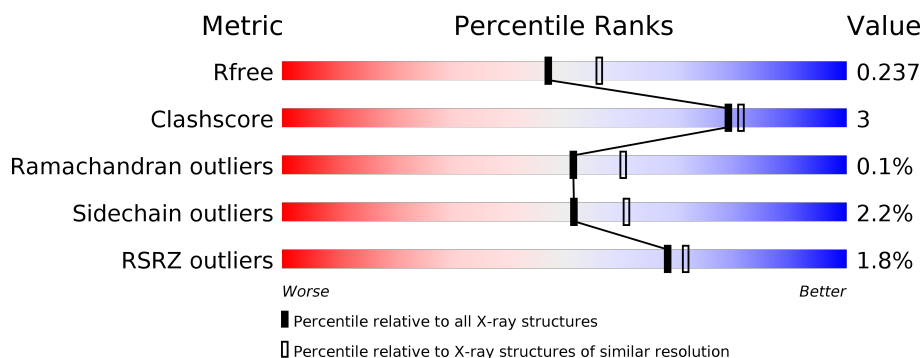
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 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	331	<div> <div>87%</div> <div>8%</div> <div>••</div> </div>
1	B	331	<div>3%</div> <div>87%</div> <div>9%</div> <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
3	CL	A	503	-	-	X	-
3	CL	E	503	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15744 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2436	1565	412	451	8			
1	B	319	Total	C	N	O	S	0	0	0
			2426	1559	409	450	8			
1	C	322	Total	C	N	O	S	0	1	0
			2449	1576	414	451	8			
1	D	319	Total	C	N	O	S	0	0	0
			2428	1560	410	450	8			
1	E	320	Total	C	N	O	S	0	1	0
			2451	1575	416	452	8			
1	F	321	Total	C	N	O	S	0	0	0
			2440	1569	412	451	8			

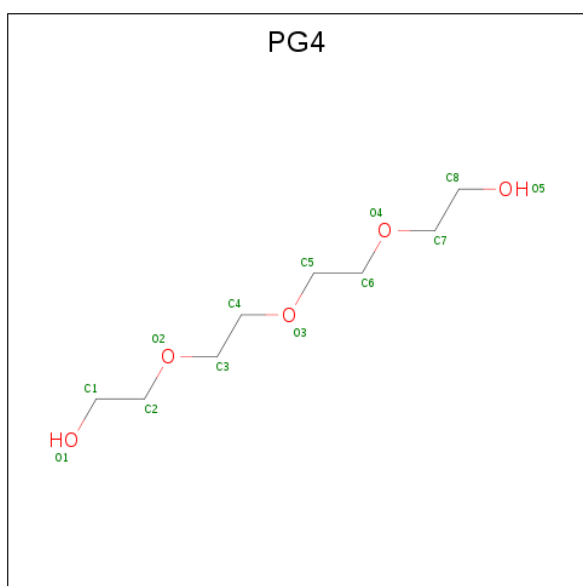
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Cu	0	0
			2	2		
2	E	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		
2	C	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		
2	F	2	Total	Cu	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	2	Total Cl 2 2	0	0
3	D	2	Total Cl 2 2	0	0
3	E	1	Total Cl 1 1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 6 3	0	0
4	A	1	Total C O 9 6 3	0	0
4	E	1	Total C O 10 6 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	150	Total O 151 151	0	1
5	B	161	Total O 162 162	0	1
5	C	186	Total O 188 188	0	2

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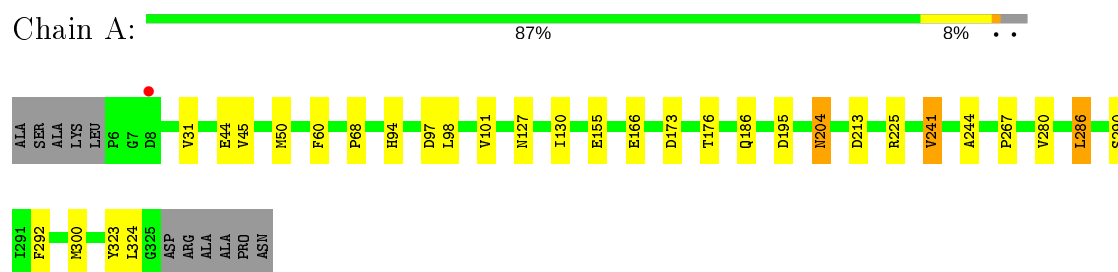
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	184	Total 184	O 184	0	0
5	E	205	Total 205	O 205	0	0
5	F	176	Total 178	O 178	0	2

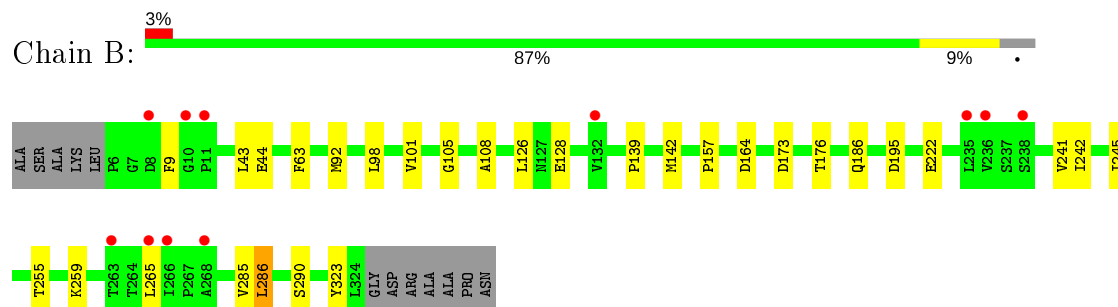
### 3 Residue-property plots [i](#)

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.

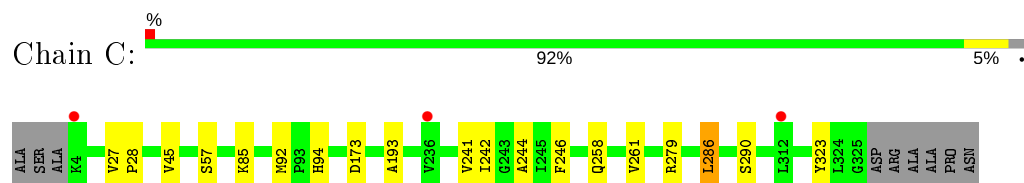
- Molecule 1: Copper-containing nitrite reductase



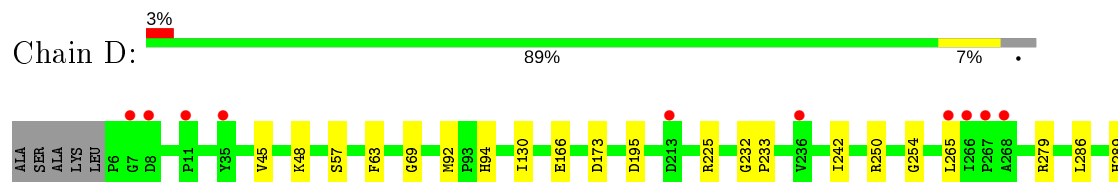
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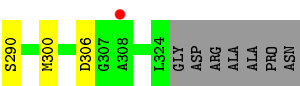


- Molecule 1: Copper-containing nitrite reductase

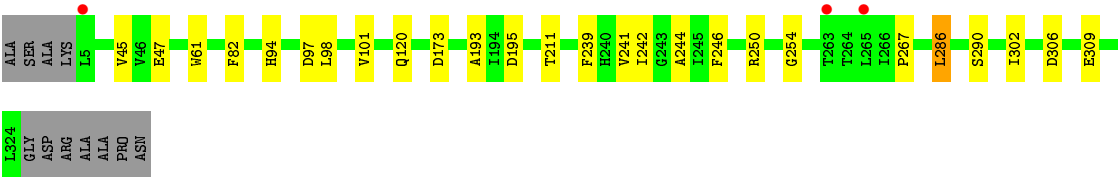
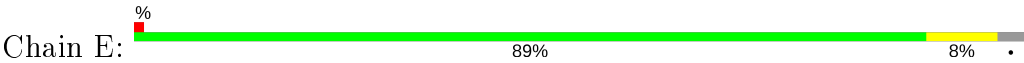


- Molecule 1: Copper-containing nitrite reductase

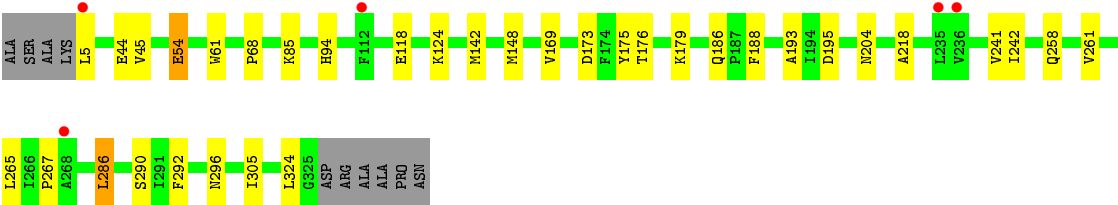
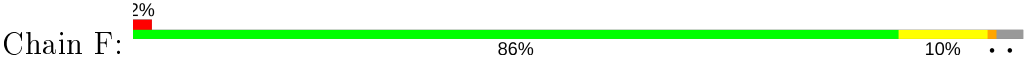




● Molecule 1: Copper-containing nitrite reductase



● Molecule 1: Copper-containing nitrite reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.88Å 167.52Å 143.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.68 – 2.25 42.64 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.1 (42.68-2.25) 94.1 (42.64-2.25)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.179 , 0.237 0.184 , 0.237	Depositor DCC
$R_{free}$ test set	4426 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.065 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: PG4, CU, CL

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	0.65	0/2504	0.82	0/3403
1	B	0.65	0/2494	0.82	0/3392
1	C	0.66	0/2520	0.83	0/3427
1	D	0.66	0/2496	0.82	0/3394
1	E	0.66	0/2519	0.83	0/3424
1	F	0.65	0/2508	0.81	0/3410
All	All	0.65	0/15041	0.82	0/20450

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	0	2
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	290	SER	Peptide
1	B	290	SER	Peptide
1	C	290	SER	Peptide
1	D	289	HIS	Peptide

## 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	2436	0	2392	17	0
1	B	2426	0	2371	18	0
1	C	2449	0	2409	13	0
1	D	2428	0	2378	11	0
1	E	2451	0	2411	15	0
1	F	2440	0	2396	18	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	2	0	0	2	0
3	B	1	0	0	1	0
3	D	2	0	0	2	0
3	E	1	0	0	2	0
4	A	18	0	22	0	0
4	E	10	0	13	0	0
5	A	151	0	0	0	0
5	B	162	0	0	1	0
5	C	188	0	0	0	0
5	D	184	0	0	0	0
5	E	205	0	0	0	0
5	F	178	0	0	0	0
All	All	15744	0	14392	81	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 3.

The worst 5 of 81 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:250:ARG:HD2	1:D:254:GLY:O	1.84	0.78
1:C:241[A]:VAL:HG13	1:C:244:ALA:HB3	1.67	0.75
1:E:97:ASP:OD2	3:E:503:CL:CL	2.50	0.67
1:F:45:VAL:HG11	1:F:94:HIS:CD2	2.30	0.66
3:B:503:CL:CL	1:C:242:ILE:HG12	2.36	0.63

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	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
1	B	317/331 (96%)	310 (98%)	7 (2%)	0	100	100
1	C	321/331 (97%)	315 (98%)	6 (2%)	0	100	100
1	D	317/331 (96%)	310 (98%)	7 (2%)	0	100	100
1	E	319/331 (96%)	315 (99%)	4 (1%)	0	100	100
1	F	319/331 (96%)	308 (97%)	10 (3%)	1 (0%)	41	46
All	All	1911/1986 (96%)	1867 (98%)	43 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	54	GLU

### 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	257/264 (97%)	250 (97%)	7 (3%)	44	54
1	B	255/264 (97%)	251 (98%)	4 (2%)	62	73
1	C	258/264 (98%)	254 (98%)	4 (2%)	62	73
1	D	256/264 (97%)	250 (98%)	6 (2%)	50	59
1	E	259/264 (98%)	254 (98%)	5 (2%)	57	66
1	F	257/264 (97%)	249 (97%)	8 (3%)	40	49
All	All	1542/1584 (97%)	1508 (98%)	34 (2%)	52	61

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	48	LYS
1	D	195	ASP
1	F	195	ASP
1	D	92	MET
1	A	324	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	127	ASN
1	D	127	ASN
1	E	260	ASN
1	C	51	GLN
1	E	127	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 21 ligands modelled in this entry, 18 are monoatomic - leaving 3 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	$\# Z  > 2$
4	PG4	A	505	-	8,8,12	0.31	0	7,7,11	0.18	0
4	PG4	E	504	-	9,9,12	0.23	0	8,8,11	0.19	0
4	PG4	A	506	-	8,8,12	0.31	0	7,7,11	0.14	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
4	PG4	A	505	-	-	3/6/6/10	-
4	PG4	E	504	-	-	1/7/7/10	-
4	PG4	A	506	-	-	3/6/6/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	504	PG4	O2-C3-C4-O3
4	A	505	PG4	C6-C5-O3-C4
4	A	506	PG4	O2-C3-C4-O3
4	A	505	PG4	C4-C3-O2-C2
4	A	506	PG4	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	320/331 (96%)	-0.35	1 (0%) 94 94	19, 30, 43, 65	0
1	B	319/331 (96%)	0.06	11 (3%) 45 47	22, 33, 51, 70	0
1	C	322/331 (97%)	-0.32	3 (0%) 84 85	20, 28, 48, 89	0
1	D	319/331 (96%)	0.04	11 (3%) 45 47	21, 32, 51, 71	0
1	E	320/331 (96%)	-0.32	3 (0%) 84 85	20, 28, 42, 83	0
1	F	321/331 (96%)	-0.29	5 (1%) 72 74	21, 32, 48, 67	0
All	All	1921/1986 (96%)	-0.20	34 (1%) 68 71	19, 31, 48, 89	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	35	TYR	3.7
1	E	5	LEU	3.6
1	B	11	PRO	3.5
1	F	236	VAL	3.5
1	B	8	ASP	3.3

### 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 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	PG4	A	506	9/13	0.66	0.23	57,61,62,63	0
4	PG4	E	504	10/13	0.87	0.17	39,46,47,47	0
4	PG4	A	505	9/13	0.90	0.18	36,37,38,38	0
3	CL	D	504	1/1	0.93	0.12	51,51,51,51	0
3	CL	B	503	1/1	0.96	0.13	50,50,50,50	0
3	CL	E	503	1/1	0.97	0.05	49,49,49,49	0
3	CL	D	503	1/1	0.97	0.10	45,45,45,45	0
3	CL	A	503	1/1	0.98	0.08	51,51,51,51	0
3	CL	A	504	1/1	0.99	0.10	48,48,48,48	0
2	CU	A	501	1/1	0.99	0.03	30,30,30,30	0
2	CU	D	501	1/1	0.99	0.02	28,28,28,28	0
2	CU	F	502	1/1	0.99	0.03	30,30,30,30	0
2	CU	F	501	1/1	1.00	0.02	33,33,33,33	0
2	CU	A	502	1/1	1.00	0.03	30,30,30,30	0
2	CU	E	501	1/1	1.00	0.03	26,26,26,26	0
2	CU	C	502	1/1	1.00	0.02	25,25,25,25	0
2	CU	B	502	1/1	1.00	0.03	30,30,30,30	0
2	CU	D	502	1/1	1.00	0.02	28,28,28,28	0
2	CU	B	501	1/1	1.00	0.02	30,30,30,30	0
2	CU	E	502	1/1	1.00	0.03	27,27,27,27	0
2	CU	C	501	1/1	1.00	0.02	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.