



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 04:53 pm BST

PDB ID : 2O5P  
Title : Crystal structure of the full length ferric pyoverdine outer membrane receptor FpvA of Pseudomonas aeruginosa in its apo form  
Authors : Cobessi, D.  
Deposited on : 2006-12-06  
Resolution : 2.77 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 : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

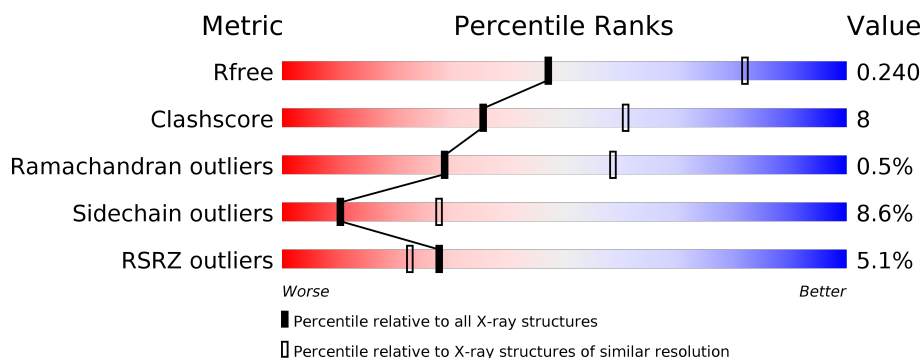
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	772	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>•</div> </div> </div>
1	B	772	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12184 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 Ferripyoverdine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	0	0	0
			6115	3845	1046	1212	12			
1	B	754	Total	C	N	O	S	0	0	0
			5995	3775	1027	1182	11			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



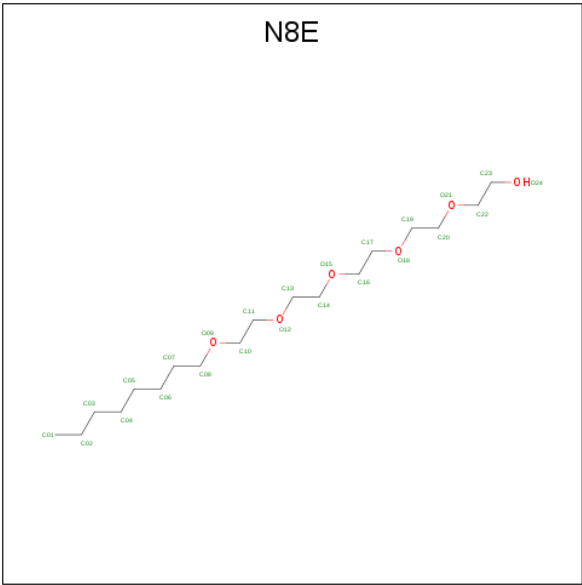
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 3 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: N8E) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>6</sub>).

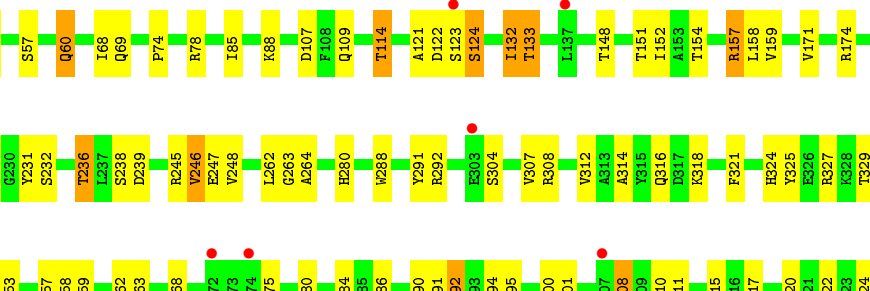


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	18	6		

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.

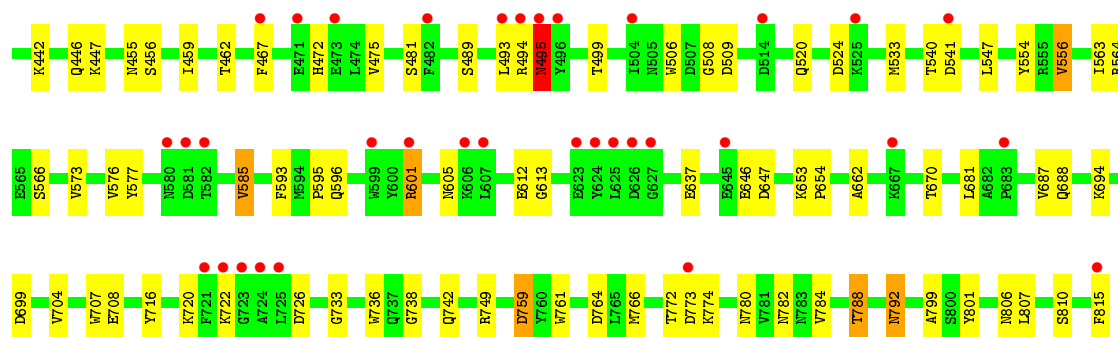
- Chain A: 

74% 23%



Index	Value	Category
E708	1563	Green
Q#4	204	Yellow
E712	1564	Green
E45	205	Yellow
Q713	1565	Green
E46	206	Yellow
Q714	1566	Green
E47	207	Yellow
Q715	1567	Green
E48	208	Yellow
Q716	1568	Green
E49	209	Yellow
Q717	1569	Green
E50	210	Yellow
Q718	1570	Green
E51	211	Yellow
Q719	1571	Green
E52	212	Yellow
Q720	1572	Green
E53	213	Yellow
Q721	1573	Green
E54	214	Yellow
Q722	1574	Green
E55	215	Yellow
Q723	1575	Green
E56	216	Yellow
Q724	1576	Green
E57	217	Yellow
Q725	1577	Green
E58	218	Yellow
Q726	1578	Green
E59	219	Yellow
Q727	1579	Green
E60	220	Yellow
Q728	1580	Green
E61	221	Yellow
Q729	1581	Green
E62	222	Yellow
Q730	1582	Green
E63	223	Yellow
Q731	1583	Green
E64	224	Yellow
Q732	1584	Green
E65	225	Yellow
Q733	1585	Green
E66	226	Yellow
Q734	1586	Green
E67	227	Yellow
Q735	1587	Green
E68	228	Yellow
Q736	1588	Green
E69	229	Yellow
Q737	1589	Green
E70	230	Yellow
Q738	1590	Green
E71	231	Yellow
Q739	1591	Green
E72	232	Yellow
Q740	1592	Green
E73	233	Yellow
Q741	1593	Green
E74	234	Yellow
Q742	1594	Green
E75	235	Yellow
Q743	1595	Green
E76	236	Yellow
Q744	1596	Green
E77	237	Yellow
Q745	1597	Green
E78	238	Yellow
Q746	1598	Green
E79	239	Yellow
Q747	1599	Green
E80	240	Yellow
Q748	1600	Green
E81	241	Yellow
Q749	1601	Green
E82	242	Yellow
Q750	1602	Green
E83	243	Yellow
Q751	1603	Green
E84	244	Yellow
Q752	1604	Green
E85	245	Yellow
Q753	1605	Green
E86	246	Yellow
Q754	1606	Green
E87	247	Yellow
Q755	1607	Green
E88	248	Yellow
Q756	1608	Green
E89	249	Yellow
Q757	1609	Green
E90	250	Yellow
Q758	1610	Green
E91	251	Yellow
Q759	1611	Green
E92	252	Yellow
Q760	1612	Green
E93	253	Yellow
Q761	1613	Green
E94	254	Yellow
Q762	1614	Green
E95	255	Yellow
Q763	1615	Green
E96	256	Yellow
Q764	1616	Green
E97	257	Yellow
Q765	1617	Green
E98	258	Yellow
Q766	1618	Green
E99	259	Yellow
Q767	1619	Green
E100	260	Yellow
Q768	1620	Green
E101	261	Yellow
Q769	1621	Green
E102	262	Yellow
Q770	1622	Green
E103	263	Yellow
Q771	1623	Green
E104	264	Yellow
Q772	1624	Green
E105	265	Yellow
Q773	1625	Green
E106	266	Yellow
Q774	1626	Green
E107	267	Yellow
Q775	1627	Green
E108	268	Yellow
Q776	1628	Green
E109	269	Yellow
Q777	1629	Green
E110	270	Yellow
Q778	1630	Green
E111	271	Yellow
Q779	1631	Green
E112	272	Yellow
Q780</		

- [illegible]



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.88Å 128.78Å 139.15Å 90.00° 130.55° 90.00°	Depositor
Resolution (Å)	30.47 – 2.77 30.47 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.47-2.77) 97.5 (30.47-2.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	8.00	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.208 , 0.247 0.203 , 0.240	Depositor DCC
$R_{free}$ test set	3195 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: N8E, PO4

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	0.59	0/6267	0.72	2/8514 (0.0%)
1	B	0.52	0/6146	0.65	0/8347
All	All	0.56	0/12413	0.68	2/16861 (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	A	687	VAL	CB-CA-C	-6.05	99.90	111.40
1	A	713	LEU	CA-CB-CG	5.08	126.99	115.30

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	6115	0	5788	114	0
1	B	5995	0	5675	79	0
2	A	30	0	0	2	0
2	B	20	0	0	0	0
3	A	24	0	38	0	0
All	All	12184	0	11501	191	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 8.

The worst 5 of 191 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:B:772:THR:HG22	1:B:774:LYS:H	1.02	1.11
1:A:772:THR:HG21	1:B:291:TYR:OH	1.64	0.96
1:A:772:THR:HG22	1:A:774:LYS:H	1.33	0.90
1:A:694:LYS:HE3	1:A:708:GLU:OE1	1.73	0.89
1:B:772:THR:HG22	1:B:774:LYS:N	1.88	0.88

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	770/772 (100%)	724 (94%)	41 (5%)	5 (1%)	25	54
1	B	750/772 (97%)	717 (96%)	30 (4%)	3 (0%)	34	64
All	All	1520/1544 (98%)	1441 (95%)	71 (5%)	8 (0%)	29	58

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	SER
1	A	121	ALA
1	B	407	ALA
1	B	495	ASN
1	A	122	ASP

### 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	650/650 (100%)	592 (91%)	58 (9%)	9	26
1	B	637/650 (98%)	584 (92%)	53 (8%)	11	29
All	All	1287/1300 (99%)	1176 (91%)	111 (9%)	10	28

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	744	VAL
1	B	96	THR
1	B	722	LYS
1	A	766	MET
1	A	811	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	615	ASN
1	B	176	ASN
1	B	742	GLN
1	A	642	ASN
1	B	109	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

11 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	PO4	A	9	-	4,4,4	0.88	0	6,6,6	0.43	0
2	PO4	B	2	-	4,4,4	0.80	0	6,6,6	0.83	0
2	PO4	A	4	-	4,4,4	0.95	0	6,6,6	0.72	0
2	PO4	B	6	-	4,4,4	0.92	0	6,6,6	0.51	0
2	PO4	B	8	-	4,4,4	0.89	0	6,6,6	0.48	0
2	PO4	A	7	-	4,4,4	0.85	0	6,6,6	0.52	0
2	PO4	B	5	-	4,4,4	0.75	0	6,6,6	0.81	0
2	PO4	A	3	-	4,4,4	0.97	0	6,6,6	0.45	0
2	PO4	A	1	-	4,4,4	0.97	0	6,6,6	1.18	0
2	PO4	A	10	-	4,4,4	1.03	0	6,6,6	0.42	0
3	N8E	A	11	-	23,23,23	0.78	1 (4%)	22,22,22	0.48	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
3	N8E	A	11	-	-	11/21/21/21	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	11	N8E	C04-C03	-3.01	1.34	1.51

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

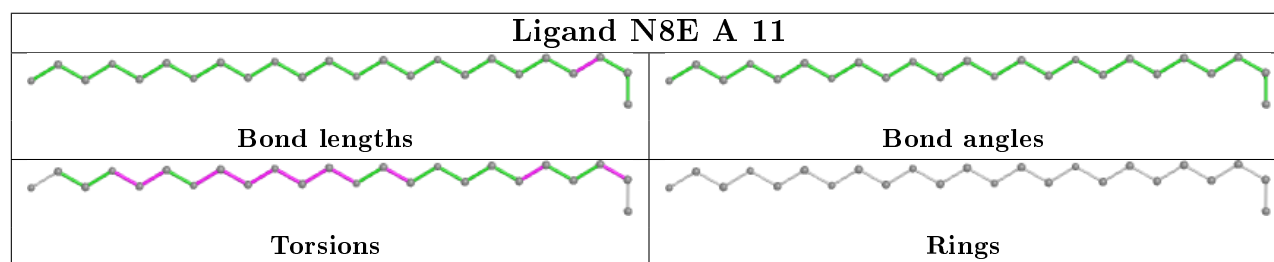
Mol	Chain	Res	Type	Atoms
3	A	11	N8E	O09-C10-C11-O12
3	A	11	N8E	O12-C13-C14-O15
3	A	11	N8E	C01-C02-C03-C04
3	A	11	N8E	C13-C14-O15-C16
3	A	11	N8E	C17-C16-O15-C14

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4	PO4	1	0
2	A	10	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

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	772/772 (100%)	0.15	21 (2%)	54 49	32, 40, 48, 55	0
1	B	754/772 (97%)	0.37	57 (7%)	13 9	31, 40, 46, 53	0
All	All	1526/1544 (98%)	0.26	78 (5%)	28 22	31, 40, 47, 55	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	ALA	7.1
1	B	44	GLN	5.0
1	B	723	GLY	4.6
1	B	343	ASP	4.6
1	A	407	ALA	4.5

### 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](#)

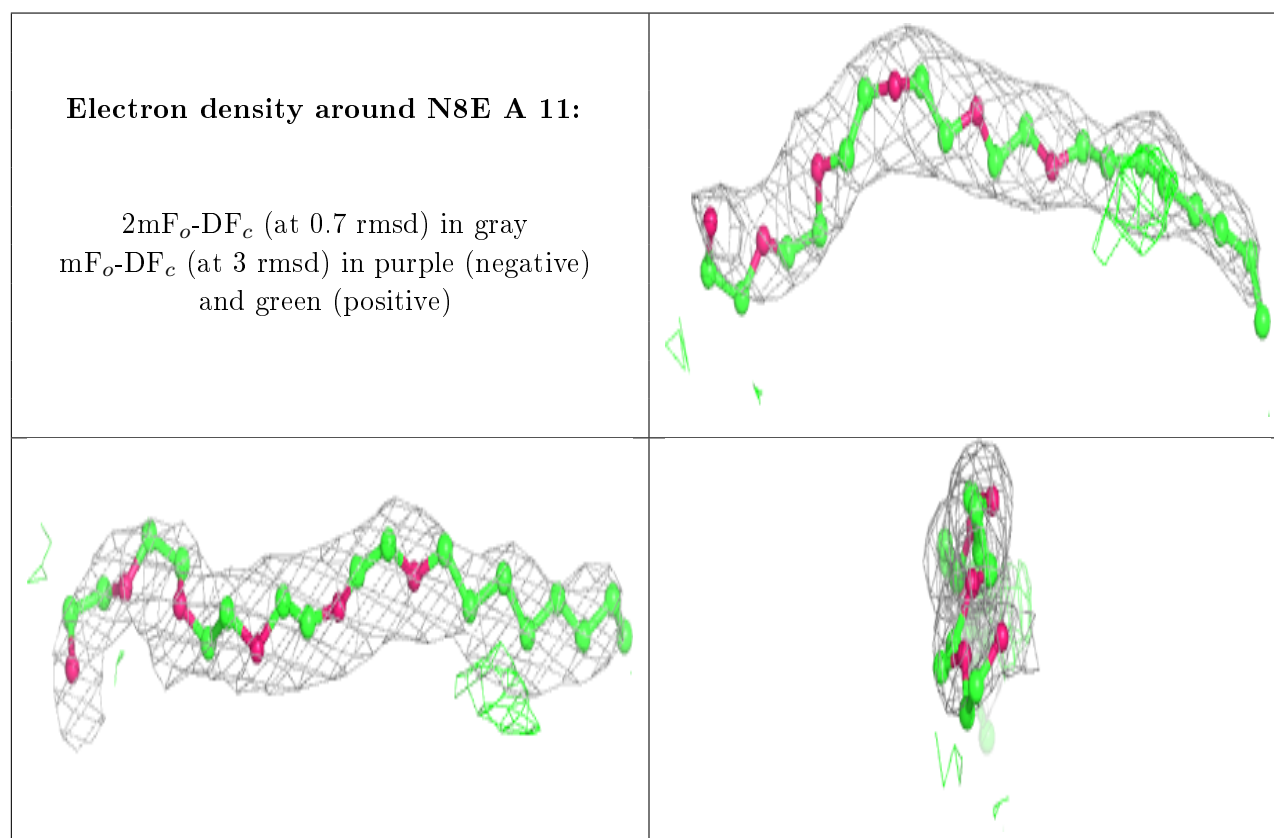
There are no carbohydrates in this entry.

### 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. 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
3	N8E	A	11	24/24	0.77	0.31	66,75,80,80	0
2	PO4	B	8	5/5	0.92	0.30	84,85,85,86	0
2	PO4	A	7	5/5	0.93	0.32	68,69,69,70	0
2	PO4	B	2	5/5	0.95	0.38	75,76,76,77	0
2	PO4	A	10	5/5	0.95	0.26	68,69,69,70	0
2	PO4	A	9	5/5	0.95	0.25	74,74,75,76	0
2	PO4	B	6	5/5	0.96	0.18	66,66,66,68	0
2	PO4	A	1	5/5	0.98	0.15	48,48,49,50	0
2	PO4	B	5	5/5	0.98	0.10	48,49,49,50	0
2	PO4	A	3	5/5	0.98	0.09	50,50,50,50	0
2	PO4	A	4	5/5	0.99	0.15	50,51,52,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.