



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 03:13 am BST

PDB ID : 6MFY
Title : Crystal structure of a 5-domain construct of LgrA in the substrate donation state
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Deposited on : 2018-09-12
Resolution : 2.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

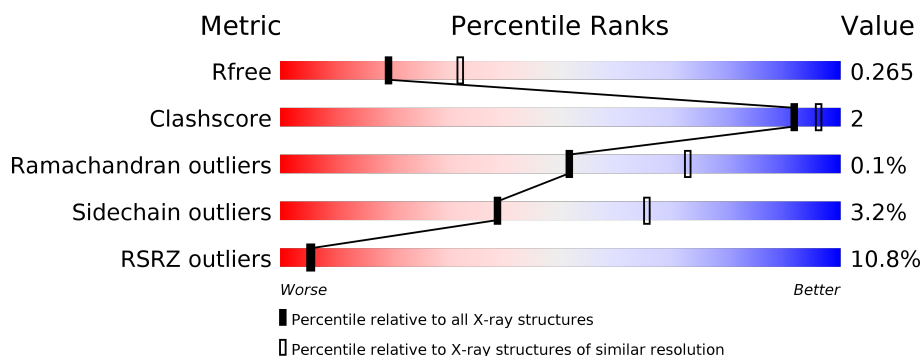
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	1728	<div> <div>10%</div> <div>87%</div> <div>5% • 8%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12865 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.

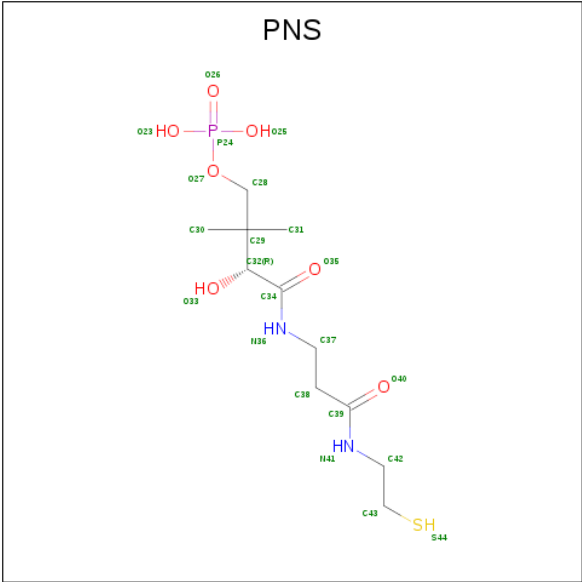
- Molecule 1 is a protein called Linear gramicidin synthase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1598	Total	C	N	O	S	0	0	0
			12694	8108	2164	2367	55			

There are 13 discrepancies between the modelled and reference sequences:

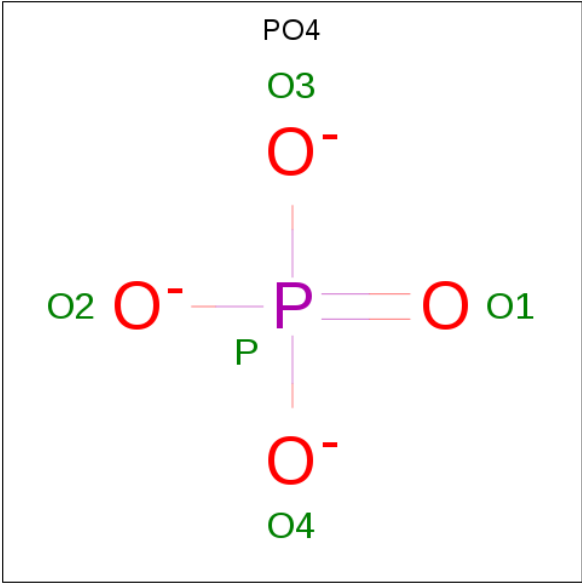
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q70LM7
A	0	ALA	-	expression tag	UNP Q70LM7
A	1	MET	-	expression tag	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	1718	ALA	-	expression tag	UNP Q70LM7
A	1719	ALA	-	expression tag	UNP Q70LM7
A	1720	ALA	-	expression tag	UNP Q70LM7
A	1721	GLU	-	expression tag	UNP Q70LM7
A	1722	ASN	-	expression tag	UNP Q70LM7
A	1723	LEU	-	expression tag	UNP Q70LM7
A	1724	TYR	-	expression tag	UNP Q70LM7
A	1725	PHE	-	expression tag	UNP Q70LM7
A	1726	GLN	-	expression tag	UNP Q70LM7

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C₁₁H₂₃N₂O₇PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

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

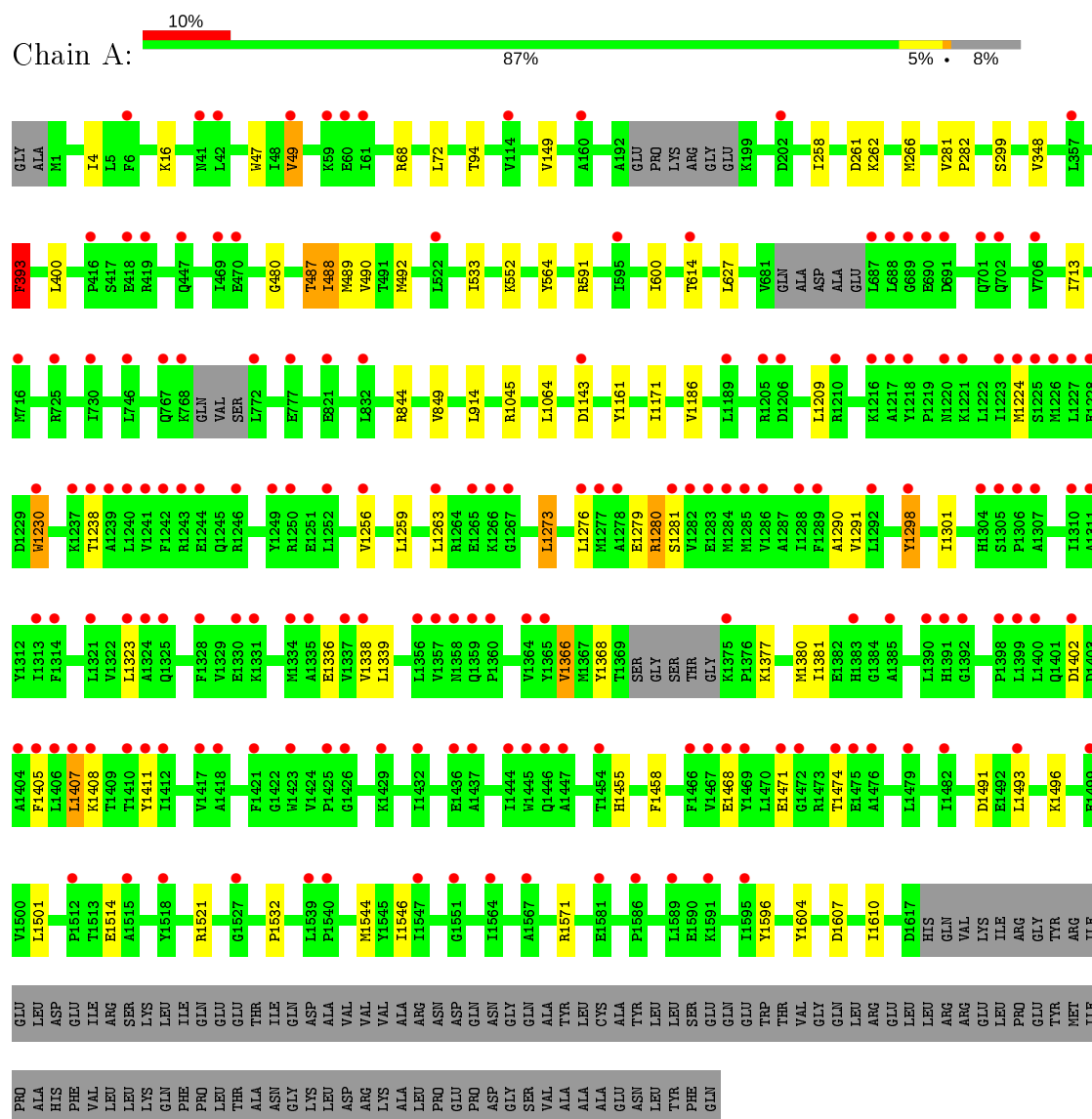
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	0
			100	100		

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: Linear gramicidin synthase subunit A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.86Å 141.11Å 171.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.77 – 2.50 108.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (85.77-2.50) 99.5 (108.98-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.52Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.238 , 0.266 0.237 , 0.265	Depositor DCC
R_{free} test set	3793 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12865	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PNS, 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	0.50	0/12976	0.60	2/17619 (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	393	PHE	CB-CA-C	6.84	124.08	110.40
1	A	1280	ARG	CB-CA-C	5.37	121.14	110.40

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	12694	0	12562	40	0
2	A	21	0	21	0	0
3	A	50	0	0	0	0
4	A	100	0	0	1	0
All	All	12865	0	12583	40	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 2.

All (40) 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:1259:LEU:HD23	1:A:1259:LEU:O	1.84	0.77
1:A:1273:LEU:HD21	1:A:1366:VAL:HG21	1.67	0.75
1:A:1161:TYR:CG	1:A:1171:ILE:HG13	2.22	0.73
1:A:1161:TYR:CD1	1:A:1171:ILE:HG13	2.26	0.71
1:A:262:LYS:HA	1:A:266:MET:SD	2.36	0.66
1:A:258:ILE:O	1:A:393:PHE:HZ	1.82	0.62
1:A:489:MET:SD	1:A:492:MET:HE1	2.39	0.62
1:A:1366:VAL:O	1:A:1366:VAL:HG12	2.02	0.59
1:A:1230:TRP:HA	1:A:1230:TRP:CE3	2.36	0.59
1:A:1291:VAL:HG11	1:A:1298:TYR:HB3	1.83	0.59
1:A:261:ASP:O	1:A:266:MET:HE3	2.02	0.59
1:A:1280:ARG:HD2	1:A:1407:LEU:HD22	1.85	0.57
1:A:1323:LEU:HD23	1:A:1339:LEU:HB2	1.85	0.57
1:A:1546:ILE:HD12	1:A:1604:TYR:CD2	2.41	0.56
1:A:400:LEU:C	1:A:400:LEU:HD23	2.26	0.56
1:A:1263:LEU:HD21	1:A:1323:LEU:HD21	1.87	0.55
1:A:487:THR:HG22	1:A:488:ILE:HD12	1.89	0.55
1:A:1230:TRP:HA	1:A:1230:TRP:HE3	1.72	0.54
1:A:282:PRO:HD2	4:A:1953:HOH:O	2.08	0.54
1:A:552:LYS:HB3	1:A:564:TYR:CE1	2.43	0.53
1:A:489:MET:SD	1:A:492:MET:CE	2.97	0.52
1:A:914:LEU:HB3	1:A:1045:ARG:NH2	2.24	0.52
1:A:1532:PRO:HG2	1:A:1532:PRO:O	2.10	0.52
1:A:282:PRO:HD2	1:A:348:VAL:O	2.11	0.51
1:A:281:VAL:HG21	1:A:299:SER:HB2	1.94	0.50
1:A:49:VAL:HG22	1:A:49:VAL:O	2.11	0.50
1:A:1514:GLU:HG2	1:A:1596:TYR:CE1	2.48	0.49
1:A:614:THR:HG22	1:A:614:THR:O	2.13	0.48
1:A:49:VAL:HG23	1:A:72:LEU:HD13	1.96	0.47
1:A:4:ILE:HG12	1:A:47:TRP:HB2	1.96	0.47
1:A:261:ASP:C	1:A:266:MET:HE3	2.35	0.47
1:A:400:LEU:HD12	1:A:488:ILE:HG21	1.96	0.47
1:A:490:VAL:HG11	1:A:533:ILE:HG21	1.98	0.46
1:A:480:GLY:HA3	1:A:489:MET:SD	2.56	0.45
1:A:1279:GLU:O	1:A:1280:ARG:C	2.55	0.45
1:A:1380:MET:O	1:A:1571:ARG:N	2.50	0.45
1:A:400:LEU:HB2	1:A:488:ILE:HG21	1.98	0.45
1:A:1544:MET:SD	1:A:1610:ILE:HD12	2.57	0.44
1:A:600:ILE:CD1	1:A:627:LEU:HD13	2.47	0.44
1:A:1256:VAL:HG13	1:A:1290:ALA:HB2	2.01	0.43

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	1588/1728 (92%)	1518 (96%)	68 (4%)	2 (0%)	51 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	487	THR
1	A	488	ILE

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	1359/1490 (91%)	1315 (97%)	44 (3%)	39 65

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	49	VAL
1	A	68	ARG
1	A	94	THR
1	A	149	VAL
1	A	393	PHE

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Mol	Chain	Res	Type
1	A	591	ARG
1	A	713	ILE
1	A	844	ARG
1	A	849	VAL
1	A	1064	LEU
1	A	1143	ASP
1	A	1186	VAL
1	A	1209	LEU
1	A	1224	MET
1	A	1230	TRP
1	A	1238	THR
1	A	1273	LEU
1	A	1276	LEU
1	A	1281	SER
1	A	1298	TYR
1	A	1301	ILE
1	A	1336	GLU
1	A	1338	VAL
1	A	1366	VAL
1	A	1368	TYR
1	A	1377	LYS
1	A	1381	ILE
1	A	1402	ASP
1	A	1405	PHE
1	A	1407	LEU
1	A	1408	LYS
1	A	1411	TYR
1	A	1455	HIS
1	A	1458	PHE
1	A	1468	GLU
1	A	1471	GLU
1	A	1474	THR
1	A	1491	ASP
1	A	1493	LEU
1	A	1496	LYS
1	A	1501	LEU
1	A	1521	ARG
1	A	1607	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\# Z > 2$
3	PO4	A	1804	-	4,4,4	0.88	0	6,6,6	0.51	0
3	PO4	A	1810	-	4,4,4	0.89	0	6,6,6	0.43	0
3	PO4	A	1803	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	A	1811	-	4,4,4	0.87	0	6,6,6	0.45	0
3	PO4	A	1807	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	A	1805	-	4,4,4	0.88	0	6,6,6	0.40	0
3	PO4	A	1802	-	4,4,4	0.93	0	6,6,6	0.43	0
3	PO4	A	1809	-	4,4,4	0.90	0	6,6,6	0.41	0
3	PO4	A	1806	-	4,4,4	0.90	0	6,6,6	0.42	0
3	PO4	A	1808	-	4,4,4	0.86	0	6,6,6	0.44	0
2	PNS	A	1801	1	13,20,21	2.40	4 (30%)	18,26,29	1.44	3 (16%)

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	PNS	A	1801	1	-	3/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1801	PNS	C34-N36	5.61	1.45	1.33
2	A	1801	PNS	C39-N41	5.36	1.45	1.33
2	A	1801	PNS	O35-C34	-2.20	1.19	1.23
2	A	1801	PNS	O40-C39	-2.10	1.19	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1801	PNS	C38-C39-N41	2.89	121.29	116.42
2	A	1801	PNS	C37-C38-C39	-2.56	108.10	112.36
2	A	1801	PNS	C42-N41-C39	-2.41	118.36	122.84

There are no chirality outliers.

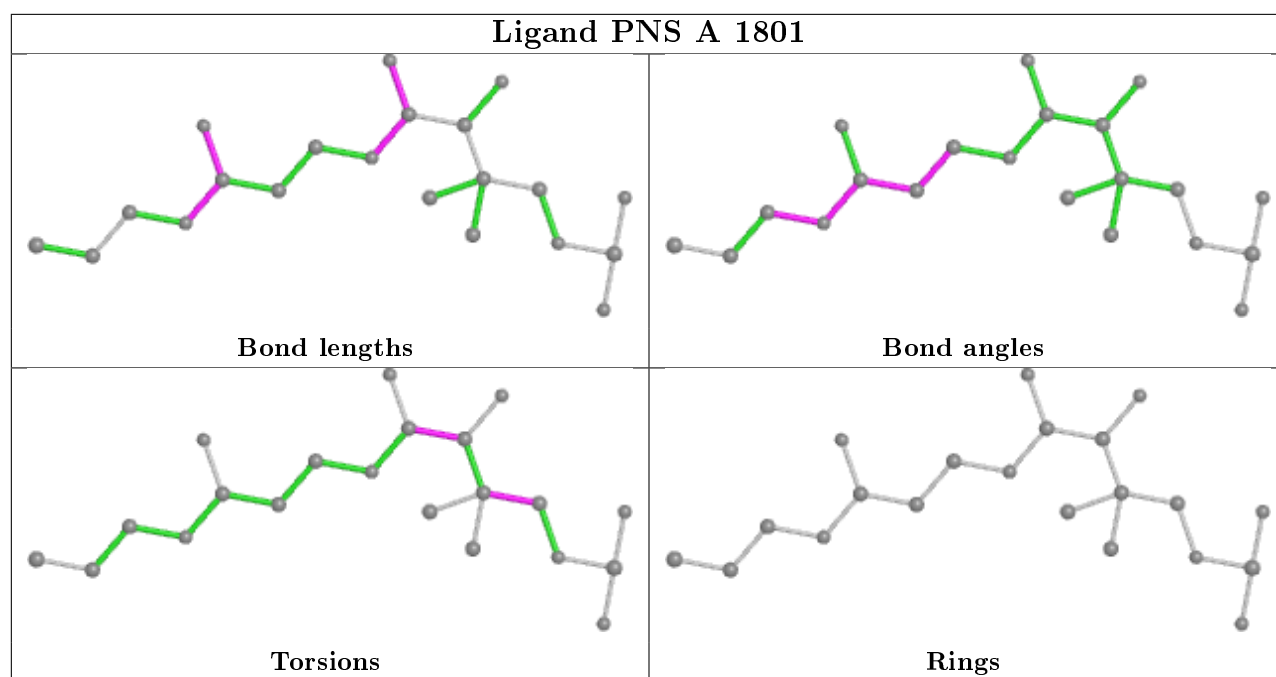
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1801	PNS	O27-C28-C29-C31
2	A	1801	PNS	O33-C32-C34-N36
2	A	1801	PNS	O27-C28-C29-C30

There are no ring outliers.

No monomer is involved in short contacts.

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 [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, 95th 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 ²)	Q<0.9
1	A	1598/1728 (92%)	0.87	172 (10%) 5 5	37, 61, 153, 184	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1285	MET	8.2
1	A	1444	ILE	8.0
1	A	1292	LEU	7.0
1	A	1304	HIS	6.8
1	A	1226	MET	6.2
1	A	1356	LEU	6.0
1	A	1437	ALA	5.9
1	A	1238	THR	5.9
1	A	1323	LEU	5.8
1	A	1278	ALA	5.6
1	A	1282	VAL	5.5
1	A	1298	TYR	5.4
1	A	1307	ALA	5.4
1	A	1436	GLU	5.3
1	A	1305	SER	5.3
1	A	1471	GLU	5.3
1	A	1244	GLU	5.2
1	A	1423	TRP	5.1
1	A	1277	MET	5.0
1	A	1330	GLU	5.0
1	A	1224	MET	5.0
1	A	1432	ILE	4.9
1	A	1411	TYR	4.9
1	A	1283	GLU	4.8
1	A	1426	GLY	4.8
1	A	1225	SER	4.8
1	A	1359	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	1267	GLY	4.7
1	A	1482	ILE	4.7
1	A	1252	LEU	4.6
1	A	1328	PHE	4.6
1	A	1567	ALA	4.6
1	A	1221	LYS	4.5
1	A	1417	VAL	4.4
1	A	1249	TYR	4.3
1	A	1589	LEU	4.3
1	A	1220	ASN	4.3
1	A	767	GLN	4.0
1	A	1240	LEU	4.0
1	A	1216	LYS	3.9
1	A	1143	ASP	3.9
1	A	1284	MET	3.9
1	A	1289	PHE	3.9
1	A	1265	GLU	3.9
1	A	1383	HIS	3.9
1	A	772	LEU	3.9
1	A	1276	LEU	3.9
1	A	1421	PHE	3.8
1	A	1364	VAL	3.8
1	A	688	LEU	3.7
1	A	1263	LEU	3.7
1	A	1306	PRO	3.7
1	A	1591	LYS	3.7
1	A	1539	LEU	3.7
1	A	1406	LEU	3.6
1	A	1241	VAL	3.6
1	A	1313	ILE	3.5
1	A	1335	ALA	3.4
1	A	1281	SER	3.4
1	A	1499	GLU	3.4
1	A	1321	LEU	3.4
1	A	1385	ALA	3.4
1	A	1466	PHE	3.3
1	A	1425	PRO	3.3
1	A	1357	VAL	3.3
1	A	1227	LEU	3.3
1	A	1390	LEU	3.3
1	A	1475	GLU	3.3
1	A	42	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1239	ALA	3.2
1	A	1454	THR	3.2
1	A	1375	LYS	3.2
1	A	1230	TRP	3.2
1	A	1310	ILE	3.2
1	A	1518	TYR	3.1
1	A	1242	PHE	3.1
1	A	1581	GLU	3.1
1	A	1286	VAL	3.1
1	A	1479	LEU	3.1
1	A	60	GLU	3.1
1	A	1493	LEU	3.1
1	A	1358	ASN	3.0
1	A	1391	HIS	3.0
1	A	1446	GLN	2.9
1	A	1476	ALA	2.9
1	A	418	GLU	2.9
1	A	595	ILE	2.9
1	A	1405	PHE	2.9
1	A	1547	ILE	2.9
1	A	1205	ARG	2.9
1	A	1325	GLN	2.9
1	A	1334	MET	2.9
1	A	1360	PRO	2.9
1	A	1429	LYS	2.8
1	A	1228	GLU	2.8
1	A	1288	ILE	2.8
1	A	416	PRO	2.8
1	A	61	ILE	2.8
1	A	1472	GLY	2.8
1	A	1467	VAL	2.8
1	A	1412	ILE	2.7
1	A	1564	ILE	2.7
1	A	1392	GLY	2.7
1	A	1404	ALA	2.7
1	A	687	LEU	2.7
1	A	1398	PRO	2.7
1	A	777	GLU	2.7
1	A	725	ARG	2.7
1	A	1331	LYS	2.7
1	A	1527	GLY	2.7
1	A	1246	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	689	GLY	2.6
1	A	1206	ASP	2.6
1	A	1324	ALA	2.6
1	A	1595	ILE	2.6
1	A	1210	ARG	2.6
1	A	1217	ALA	2.6
1	A	1400	LEU	2.6
1	A	1512	PRO	2.6
1	A	1399	LEU	2.5
1	A	1407	LEU	2.5
1	A	1402	ASP	2.5
1	A	59	LYS	2.5
1	A	614	THR	2.5
1	A	1410	THR	2.5
1	A	1189	LEU	2.5
1	A	1256	VAL	2.5
1	A	6	PHE	2.5
1	A	1223	ILE	2.5
1	A	716	MET	2.5
1	A	690	GLU	2.5
1	A	1474	THR	2.5
1	A	1586	PRO	2.4
1	A	702	GLN	2.4
1	A	691	ASP	2.4
1	A	1250	ARG	2.4
1	A	1365	TYR	2.4
1	A	202	ASP	2.4
1	A	730	ILE	2.4
1	A	1266	LYS	2.3
1	A	706	VAL	2.3
1	A	1469	TYR	2.3
1	A	832	LEU	2.3
1	A	821	GLU	2.3
1	A	1408	LYS	2.2
1	A	1540	PRO	2.2
1	A	1445	TRP	2.2
1	A	1243	ARG	2.2
1	A	1468	GLU	2.2
1	A	160	ALA	2.2
1	A	701	GLN	2.2
1	A	768	LYS	2.2
1	A	1311	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1447	ALA	2.2
1	A	114	VAL	2.2
1	A	522	LEU	2.1
1	A	1337	VAL	2.1
1	A	41	ASN	2.1
1	A	470	GLU	2.1
1	A	49	VAL	2.1
1	A	1218	TYR	2.1
1	A	419	ARG	2.1
1	A	746	LEU	2.1
1	A	1418	ALA	2.1
1	A	1338	VAL	2.0
1	A	1237	LYS	2.0
1	A	1551	GLY	2.0
1	A	447	GLN	2.0
1	A	1515	ALA	2.0
1	A	357	LEU	2.0
1	A	469	ILE	2.0
1	A	1314	PHE	2.0

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, 95th 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.

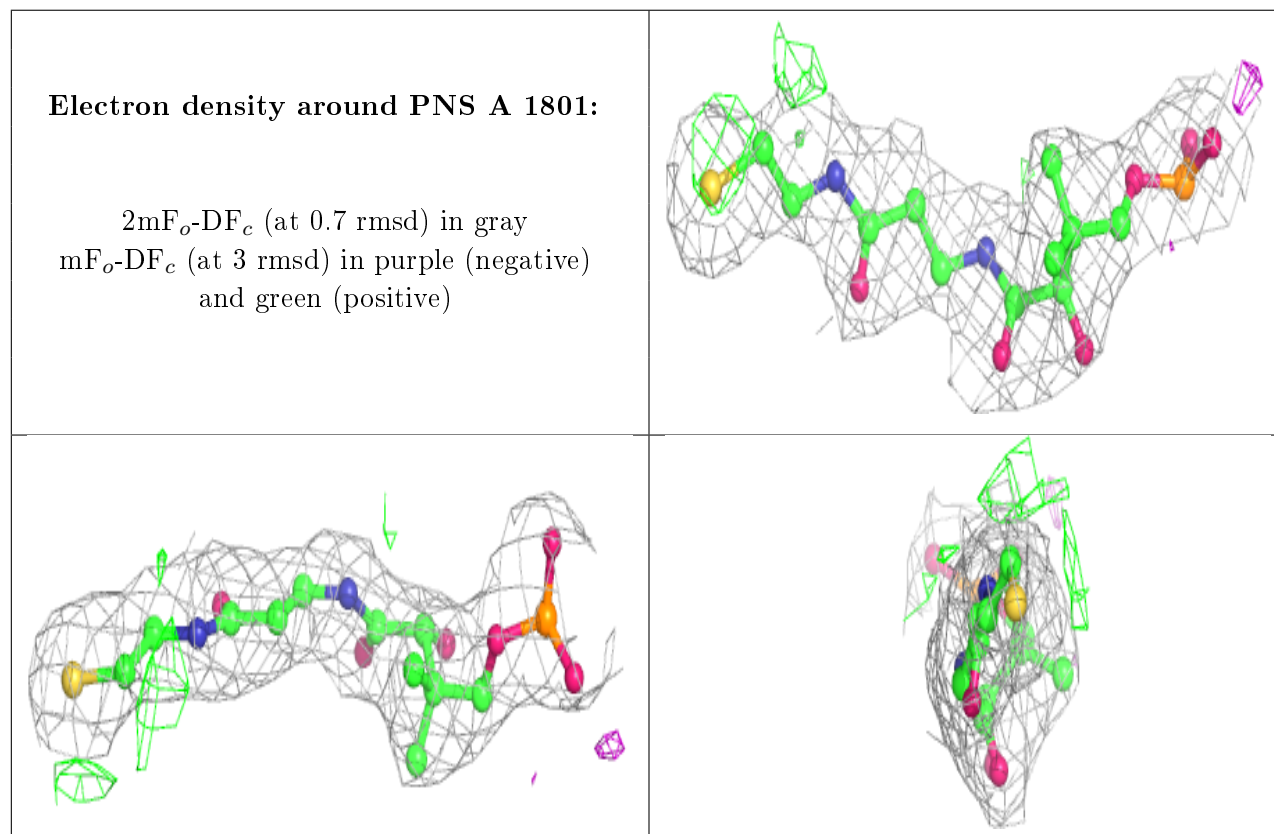
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	A	1808	5/5	0.64	0.23	82,83,85,85	0
3	PO4	A	1806	5/5	0.76	0.23	82,82,83,83	0
3	PO4	A	1804	5/5	0.78	0.22	82,83,85,89	0
3	PO4	A	1811	5/5	0.83	0.30	80,80,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	A	1805	5/5	0.83	0.24	82,83,85,87	0
3	PO4	A	1807	5/5	0.85	0.16	80,81,83,89	0
3	PO4	A	1810	5/5	0.88	0.33	80,86,88,89	0
3	PO4	A	1809	5/5	0.90	0.38	83,85,87,88	0
3	PO4	A	1803	5/5	0.91	0.21	80,81,83,83	0
2	PNS	A	1801	21/22	0.96	0.15	45,48,53,56	0
3	PO4	A	1802	5/5	0.97	0.21	50,51,58,70	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.