



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 01:30 AM EDT

PDB ID : 5ES9  
Title : Crystal structure of the LgrA initiation module in the formylation state  
Authors : Reimer, J.M.; Aloise, M.N.; Schmeing, T.M.  
Deposited on : 2015-11-16  
Resolution : 3.77 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
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) : 2.35.1

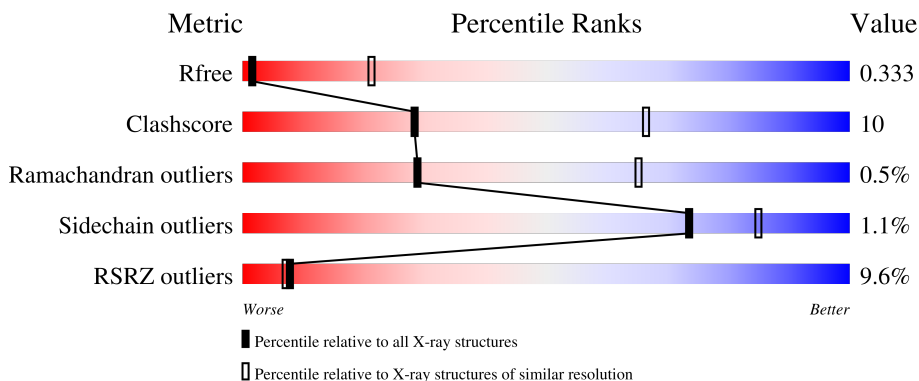
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


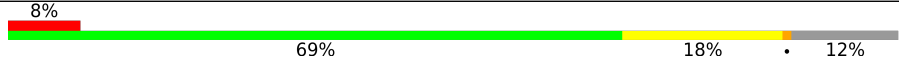
The reported resolution of this entry is 3.77 Å.

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	1038 (3.96-3.60)
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)

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 of 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	776	
1	B	776	

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	PNS	A	801	-	-	-	X

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 11509 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.

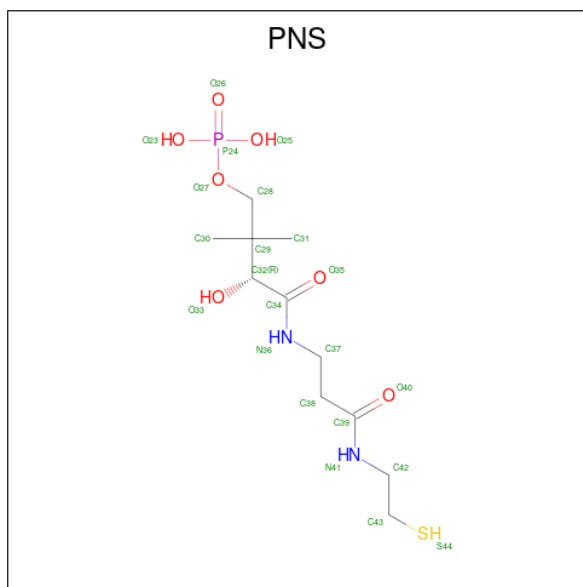
- Molecule 1 is a protein called Linear gramicidin synthetase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	759	6064	3869	1042	1126	27	0	0	0
1	B	681	5440	3473	930	1012	25	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	768	ALA	-	expression tag	UNP Q70LM7
A	769	ALA	-	expression tag	UNP Q70LM7
A	770	ALA	-	expression tag	UNP Q70LM7
A	771	GLU	-	expression tag	UNP Q70LM7
A	772	ASN	-	expression tag	UNP Q70LM7
A	773	LEU	-	expression tag	UNP Q70LM7
A	774	TYR	-	expression tag	UNP Q70LM7
A	775	PHE	-	expression tag	UNP Q70LM7
A	776	GLN	-	expression tag	UNP Q70LM7
B	1	MET	-	initiating methionine	UNP Q70LM7
B	2	GLY	-	expression tag	UNP Q70LM7
B	768	ALA	-	expression tag	UNP Q70LM7
B	769	ALA	-	expression tag	UNP Q70LM7
B	770	ALA	-	expression tag	UNP Q70LM7
B	771	GLU	-	expression tag	UNP Q70LM7
B	772	ASN	-	expression tag	UNP Q70LM7
B	773	LEU	-	expression tag	UNP Q70LM7
B	774	TYR	-	expression tag	UNP Q70LM7
B	775	PHE	-	expression tag	UNP Q70LM7
B	776	GLN	-	expression tag	UNP Q70LM7

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).



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

### 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: Linear gramicidin synthetase subunit A





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.06Å 162.06Å 206.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 3.77 48.45 – 3.46	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.45-3.77) 97.4 (48.45-3.46)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.48Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.308 , 0.331 0.312 , 0.333	Depositor DCC
$R_{free}$ test set	2013 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	188.6	Xtrriage
Anisotropy	0.201	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 198.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	0.207 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	261.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: PNS

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	0.29	0/6203	0.49	0/8418
1	B	0.26	0/5568	0.48	0/7559
All	All	0.28	0/11771	0.49	0/15977

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	LEU	Peptide

### 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	6064	0	6001	136	1
1	B	5440	0	5369	94	0
2	A	5	0	0	0	0
All	All	11509	0	11370	223	1

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 10.

All (223) 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:455:SER:O	1:B:199:LYS:NZ	2.00	0.94
1:B:453:ASN:HD21	1:B:456:PHE:H	1.19	0.91
1:A:126:LEU:HD12	1:A:177:ASN:HA	1.55	0.87
1:A:216:THR:HB	1:A:219:HIS:HD2	1.40	0.86
1:A:588:VAL:HG21	1:A:625:LYS:HD2	1.60	0.82
1:A:713:ILE:HD11	1:A:725:ARG:HG2	1.65	0.78
1:B:668:THR:HG23	1:B:674:ASP:HB3	1.64	0.78
1:A:453:ASN:HD21	1:A:456:PHE:H	1.32	0.77
1:B:199:LYS:O	1:B:510:ARG:NH2	2.19	0.76
1:B:681:VAL:HG12	1:B:682:GLN:H	1.51	0.75
1:A:199:LYS:O	1:A:510:ARG:NH2	2.19	0.75
1:A:3:ARG:NH1	1:A:43:GLN:O	2.21	0.74
1:A:652:ASP:HB2	1:A:758:ARG:HD3	1.70	0.74
1:B:482:GLY:HA3	1:B:489:MET:HA	1.68	0.74
1:A:590:ILE:HG13	1:A:627:LEU:HG	1.70	0.73
1:B:126:LEU:HD11	1:B:184:LEU:HD22	1.72	0.71
1:B:3:ARG:NH1	1:B:43:GLN:O	2.25	0.70
1:B:615:VAL:HG12	1:B:629:GLY:HA2	1.73	0.69
1:A:615:VAL:HG12	1:A:629:GLY:HA2	1.75	0.68
1:B:77:LEU:HB2	1:B:99:THR:HG21	1.76	0.68
1:A:589:LYS:HB2	1:A:593:TYR:O	1.93	0.68
1:A:648:ASN:HA	1:A:762:ARG:HH12	1.60	0.67
1:A:177:ASN:N	1:A:177:ASN:ND2	2.43	0.66
1:A:367:ASN:ND2	1:A:536:GLU:O	2.28	0.66
1:A:730:ILE:HG13	1:A:731:LYS:HD2	1.78	0.65
1:A:588:VAL:HG12	1:A:589:LYS:O	1.95	0.65
1:A:708:SER:OG	1:A:713:ILE:O	2.15	0.64
1:A:77:LEU:HD21	1:A:108:ASP:O	1.99	0.63
1:B:396:ASP:HB2	1:B:488:ILE:HG12	1.80	0.63
1:A:177:ASN:HD22	1:A:177:ASN:H	1.47	0.62
1:B:510:ARG:NH1	1:B:536:GLU:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:HIS:HB3	1:A:759:GLN:HB3	1.80	0.62
1:B:595:ILE:HG21	1:B:627:LEU:HD11	1.80	0.62
1:B:665:PHE:HD2	1:B:673:VAL:HG11	1.64	0.61
1:A:668:THR:HG23	1:A:674:ASP:HB3	1.83	0.60
1:A:740:LYS:HD3	1:A:745:SER:HB2	1.82	0.60
1:A:718:ILE:HG13	1:A:758:ARG:HB3	1.84	0.59
1:B:435:ILE:O	1:B:455:SER:OG	2.20	0.59
1:B:77:LEU:HD11	1:B:108:ASP:HB3	1.85	0.59
1:A:177:ASN:N	1:A:177:ASN:HD22	2.01	0.58
1:A:721:HIS:CD2	1:A:755:PRO:HB2	2.37	0.58
1:A:747:ARG:HB3	1:A:750:GLN:HG2	1.85	0.58
1:A:665:PHE:HD2	1:A:673:VAL:HG11	1.67	0.58
1:B:170:ARG:NH2	1:B:177:ASN:OD1	2.37	0.58
1:B:207:GLN:HG2	1:B:338:HIS:CE1	2.38	0.58
1:A:388:LEU:HD13	1:A:435:ILE:HG21	1.86	0.57
1:B:392:SER:HB3	1:B:395:PHE:CE2	2.39	0.57
1:A:454:GLN:HG2	1:B:197:GLY:HA2	1.85	0.57
1:B:76:LEU:HD12	1:B:95:PRO:HB2	1.87	0.56
1:B:379:PHE:O	1:B:457:ARG:NH1	2.38	0.56
1:A:216:THR:HB	1:A:219:HIS:CD2	2.30	0.56
1:A:442:THR:HB	1:A:464:ASP:HB2	1.88	0.56
1:A:18:VAL:HG13	1:A:28:VAL:HG11	1.88	0.55
1:B:367:ASN:HB3	1:B:487:THR:OG1	2.07	0.55
1:A:590:ILE:HB	1:A:595:ILE:HD12	1.88	0.55
1:B:610:ILE:HG22	1:B:633:ALA:HB2	1.89	0.55
1:A:219:HIS:ND1	1:B:341:ARG:HD2	2.22	0.55
1:A:758:ARG:O	1:A:762:ARG:HG3	2.08	0.54
1:B:73:HIS:ND1	1:B:75:SER:OG	2.39	0.54
1:A:106:HIS:HB2	1:A:109:THR:OG1	2.08	0.54
1:B:388:LEU:HD13	1:B:435:ILE:HG21	1.90	0.54
1:A:343:ASP:O	1:A:540:ARG:NH2	2.41	0.54
1:A:135:GLN:NE2	1:A:139:GLU:OE2	2.40	0.54
1:B:528:ALA:HA	1:B:571:ARG:HB3	1.89	0.54
1:A:303:ILE:HD13	1:A:319:ASP:HB2	1.91	0.53
1:A:721:HIS:ND1	1:A:724:GLU:OE1	2.41	0.53
1:A:736:ILE:HA	1:A:739:LEU:HG	1.90	0.53
1:A:651:PRO:HB3	1:A:756:THR:HG21	1.91	0.53
1:B:457:ARG:HD2	1:B:458:VAL:HG23	1.91	0.53
1:A:123:GLU:HG2	1:A:182:ARG:HH12	1.72	0.52
1:A:375:TYR:CD1	1:A:404:THR:HB	2.44	0.52
1:A:759:GLN:HA	1:A:762:ARG:HE	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLN:CG	1:B:197:GLY:HA2	2.40	0.52
1:A:652:ASP:HA	1:A:655:ILE:HD13	1.92	0.52
1:A:126:LEU:HD11	1:A:184:LEU:HD22	1.90	0.52
1:A:366:HIS:ND1	1:A:536:GLU:OE2	2.34	0.52
1:B:46:ASP:O	1:B:68:ARG:HD2	2.10	0.52
1:A:610:ILE:HG22	1:A:633:ALA:HB2	1.91	0.51
1:A:13:LYS:HG2	1:A:30:ILE:HG21	1.93	0.51
1:B:507:PRO:HG3	1:B:513:ILE:HD12	1.92	0.51
1:B:496:ASP:OD1	1:B:496:ASP:N	2.38	0.50
1:B:665:PHE:CD2	1:B:673:VAL:HG11	2.45	0.50
1:A:379:PHE:O	1:A:457:ARG:NH1	2.42	0.50
1:B:473:GLY:HA3	1:B:475:TYR:CE2	2.46	0.50
1:B:604:LEU:HD13	1:B:646:LEU:HD11	1.93	0.50
1:A:471:ARG:HD2	1:A:475:TYR:CE1	2.47	0.50
1:B:135:GLN:NE2	1:B:139:GLU:OE2	2.44	0.50
1:B:604:LEU:O	1:B:610:ILE:HD11	2.11	0.50
1:B:173:TYR:HB3	1:B:176:LEU:HD12	1.93	0.50
1:A:604:LEU:HD13	1:A:646:LEU:HD11	1.93	0.50
1:A:493:PHE:HB2	1:A:505:GLY:HA3	1.93	0.50
1:A:220:VAL:HB	1:B:341:ARG:HH22	1.76	0.49
1:A:728:ASP:O	1:A:732:VAL:HG13	2.12	0.49
1:A:245:LEU:HD21	1:A:305:LEU:HD11	1.93	0.49
1:A:662:MET:HE3	1:A:665:PHE:CE1	2.48	0.49
1:A:595:ILE:HG21	1:A:627:LEU:HD11	1.94	0.49
1:A:699:LEU:O	1:A:702:GLN:HG2	2.12	0.49
1:A:713:ILE:CD1	1:A:725:ARG:HG2	2.40	0.49
1:A:750:GLN:HB3	1:A:763:LEU:HD13	1.95	0.49
1:A:110:GLY:O	1:A:158:GLN:NE2	2.37	0.49
1:A:294:TYR:OH	1:A:545:ARG:NH2	2.46	0.49
1:A:732:VAL:HB	1:A:751:LEU:HD23	1.93	0.49
1:B:252:PRO:O	1:B:253:ASP:HB2	2.11	0.49
1:A:153:ILE:O	1:A:155:PRO:HD3	2.12	0.49
1:A:718:ILE:HD11	1:A:758:ARG:HD2	1.94	0.48
1:B:172:PHE:CZ	1:B:522:LEU:HG	2.48	0.48
1:A:431:ASN:HA	1:A:455:SER:HB2	1.95	0.48
1:B:471:ARG:HD2	1:B:475:TYR:CE1	2.48	0.48
1:A:633:ALA:HB3	1:A:661:HIS:HD2	1.79	0.48
1:A:170:ARG:HH21	1:A:177:ASN:HB3	1.79	0.48
1:B:86:VAL:O	1:B:89:SER:HB3	2.15	0.47
1:A:604:LEU:O	1:A:610:ILE:HD11	2.14	0.47
1:A:604:LEU:HG	1:A:613:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:LEU:HD23	1:A:751:LEU:HD22	1.97	0.47
1:B:343:ASP:O	1:B:540:ARG:NH2	2.44	0.47
1:B:73:HIS:HD1	1:B:75:SER:HG	1.62	0.47
1:B:639:HIS:HE1	1:B:643:ARG:HD2	1.79	0.47
1:A:96:LYS:HB2	1:A:118:ILE:O	2.15	0.46
1:B:59:LYS:O	1:B:62:VAL:HG12	2.15	0.46
1:A:704:ALA:HB1	1:A:716:MET:HB2	1.96	0.46
1:A:59:LYS:O	1:A:62:VAL:HG12	2.16	0.46
1:A:173:TYR:HB3	1:A:176:LEU:HD12	1.98	0.46
1:A:739:LEU:HD12	1:A:740:LYS:N	2.31	0.46
1:A:520:LEU:O	1:A:556:HIS:NE2	2.45	0.46
1:B:123:GLU:HG2	1:B:182:ARG:HH12	1.80	0.46
1:B:270:ILE:HD11	1:B:393:PHE:HE1	1.81	0.46
1:B:147:ASN:HB3	1:B:153:ILE:HD11	1.97	0.46
1:A:357:LEU:HB2	1:A:359:LYS:HZ1	1.81	0.46
1:B:15:ASN:ND2	1:B:138:GLU:OE2	2.49	0.46
1:A:652:ASP:CB	1:A:758:ARG:HD3	2.45	0.45
1:B:106:HIS:HB2	1:B:109:THR:OG1	2.17	0.45
1:A:590:ILE:HD12	1:A:626:TYR:HA	1.99	0.45
1:A:706:VAL:O	1:A:710:VAL:HG23	2.16	0.45
1:B:485:GLU:OE1	1:B:485:GLU:N	2.47	0.45
1:A:589:LYS:O	1:A:590:ILE:HG12	2.17	0.45
1:B:77:LEU:HD22	1:B:101:HIS:CG	2.52	0.45
1:A:569:ARG:HB3	1:A:581:LEU:O	2.17	0.45
1:B:672:LYS:HG2	1:B:673:VAL:HG13	1.98	0.45
1:A:678:LEU:HD12	1:A:678:LEU:HA	1.81	0.45
1:A:473:GLY:HA3	1:A:475:TYR:CE2	2.51	0.45
1:A:681:VAL:HG12	1:A:682:GLN:H	1.82	0.45
1:A:596:GLU:HA	1:A:597:PRO:HD2	1.80	0.44
1:B:245:LEU:HD21	1:B:305:LEU:HD11	1.98	0.44
1:B:573:LEU:HB2	1:B:577:ASN:O	2.17	0.44
1:B:453:ASN:OD1	1:B:455:SER:HB3	2.17	0.44
1:A:99:THR:HG21	1:A:112:ILE:HG12	1.99	0.44
1:A:450:GLN:O	1:A:472:ASN:ND2	2.51	0.44
1:A:170:ARG:NH2	1:A:177:ASN:HB3	2.31	0.44
1:A:452:ASP:HA	1:A:472:ASN:HB2	2.00	0.44
1:A:619:GLU:HG3	1:A:625:LYS:NZ	2.33	0.44
1:A:325:ASP:HA	1:A:326:PRO:HD2	1.89	0.44
1:B:596:GLU:HA	1:B:597:PRO:HD2	1.75	0.44
1:A:590:ILE:HG22	1:A:591:ARG:HB2	1.99	0.44
1:B:375:TYR:CD1	1:B:404:THR:HB	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:HIS:NE2	1:B:108:ASP:OD2	2.51	0.43
1:A:525:ILE:HG23	1:A:572:PHE:HB3	2.00	0.43
1:A:728:ASP:H	1:A:731:LYS:HB2	1.82	0.43
1:B:259:MET:HE2	1:B:285:PRO:HA	1.99	0.43
1:A:699:LEU:HB2	1:A:761:LYS:HE3	2.00	0.43
1:B:73:HIS:O	1:B:75:SER:N	2.47	0.43
1:B:341:ARG:HD3	1:B:343:ASP:OD1	2.18	0.43
1:B:405:HIS:HB3	1:B:410:ALA:HB3	2.01	0.43
1:B:681:VAL:HG12	1:B:682:GLN:N	2.28	0.43
1:A:758:ARG:HA	1:A:761:LYS:HB3	2.01	0.43
1:B:478:TYR:HB3	1:B:492:MET:SD	2.58	0.43
1:A:436:THR:HA	1:B:199:LYS:HZ1	1.84	0.43
1:A:750:GLN:HB3	1:A:763:LEU:CD1	2.49	0.43
1:B:406:LEU:HD23	1:B:406:LEU:HA	1.83	0.43
1:B:342:PRO:HA	1:B:365:HIS:HB2	2.01	0.43
1:A:71:ASN:HB3	1:A:101:HIS:NE2	2.33	0.43
1:A:724:GLU:OE1	1:A:724:GLU:N	2.52	0.43
1:A:112:ILE:O	1:A:155:PRO:HA	2.19	0.43
1:A:179:THR:CG2	1:A:184:LEU:HB2	2.49	0.43
1:A:732:VAL:O	1:A:736:ILE:HG12	2.18	0.43
1:A:732:VAL:HG11	1:A:752:PHE:HE1	1.84	0.43
1:B:252:PRO:HA	1:B:277:GLY:O	2.18	0.43
1:A:72:LEU:HD22	1:A:100:ILE:HG12	2.01	0.42
1:A:530:GLU:OE1	1:A:565:ARG:NH1	2.52	0.42
1:A:564:TYR:CE2	1:A:566:THR:HA	2.54	0.42
1:A:717:GLY:O	1:A:757:ILE:HG13	2.19	0.42
1:B:392:SER:HB3	1:B:395:PHE:CD2	2.53	0.42
1:A:763:LEU:HA	1:A:763:LEU:HD23	1.78	0.42
1:B:456:PHE:O	1:B:475:TYR:HB3	2.19	0.42
1:A:207:GLN:HG2	1:A:338:HIS:CE1	2.54	0.42
1:B:420:LYS:HG2	1:B:421:TYR:CD1	2.54	0.42
1:A:89:SER:O	1:A:96:LYS:NZ	2.46	0.42
1:A:607:HIS:CE1	1:A:609:LEU:HB2	2.54	0.42
1:B:5:LEU:HB2	1:B:45:ILE:HD12	2.02	0.42
1:B:345:LEU:HD21	1:B:362:MET:HB3	2.01	0.42
1:A:436:THR:OG1	1:A:437:ILE:HG22	2.19	0.42
1:A:703:LEU:O	1:A:706:VAL:HG12	2.20	0.42
1:B:72:LEU:HD22	1:B:100:ILE:HG12	2.01	0.42
1:A:456:PHE:O	1:A:475:TYR:HB3	2.19	0.42
1:A:17:VAL:HG13	1:A:141:PHE:CE1	2.55	0.42
1:A:419:ARG:O	1:A:426:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:PHE:CE1	1:B:403:PHE:HB3	2.55	0.42
1:A:435:ILE:H	1:A:455:SER:HG	1.67	0.41
1:A:732:VAL:HG11	1:A:752:PHE:CE1	2.55	0.41
1:B:269:SER:O	1:B:273:VAL:HG23	2.20	0.41
1:B:294:TYR:HE2	1:B:358:ALA:HB1	1.85	0.41
1:A:729:SER:O	1:A:732:VAL:HG22	2.21	0.41
1:B:534:VAL:HG22	1:B:563:MET:HG2	2.01	0.41
1:B:632:VAL:HA	1:B:662:MET:O	2.21	0.41
1:A:219:HIS:HE1	1:B:344:ASP:OD1	2.03	0.41
1:B:236:GLU:O	1:B:240:GLN:HG3	2.21	0.41
1:B:655:ILE:HA	1:B:656:PRO:HD3	1.88	0.41
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.86	0.41
1:B:493:PHE:CZ	1:B:503:PRO:HG2	2.55	0.41
1:A:284:ASP:HA	1:A:285:PRO:HD3	1.92	0.41
1:A:493:PHE:HB2	1:A:505:GLY:CA	2.49	0.41
1:B:76:LEU:O	1:B:79:TRP:N	2.54	0.41
1:B:145:TRP:O	1:B:149:VAL:HG23	2.21	0.41
1:B:392:SER:O	1:B:398:SER:HB2	2.20	0.41
1:B:512:ARG:NH2	1:B:561:GLU:OE2	2.51	0.41
1:A:627:LEU:HD23	1:A:627:LEU:HA	1.87	0.41
1:B:33:GLU:N	1:B:33:GLU:OE2	2.54	0.41
1:A:311:GLU:HG3	1:A:320:ILE:HD13	2.02	0.40
1:A:359:LYS:HD3	1:A:545:ARG:NH1	2.36	0.40
1:B:224:ASP:HB2	1:B:414:ILE:HG13	2.02	0.40
1:B:420:LYS:HG2	1:B:421:TYR:CE1	2.57	0.40
1:A:616:LEU:HD11	1:A:678:LEU:HD23	2.03	0.40
1:A:77:LEU:HB2	1:A:99:THR:CB	2.51	0.40
1:A:729:SER:OG	1:A:730:ILE:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:HIS:O	1:A:233:GLN:NE2[5_547]	2.15	0.05

## 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	753/776 (97%)	716 (95%)	33 (4%)	4 (0%)	29	65
1	B	677/776 (87%)	648 (96%)	26 (4%)	3 (0%)	34	69
All	All	1430/1552 (92%)	1364 (95%)	59 (4%)	7 (0%)	29	65

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	584	LEU
1	A	585	ASP
1	A	76	LEU
1	B	488	ILE
1	A	488	ILE
1	B	358	ALA
1	B	681	VAL

### 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	652/666 (98%)	645 (99%)	7 (1%)	73	85
1	B	584/666 (88%)	578 (99%)	6 (1%)	76	86
All	All	1236/1332 (93%)	1223 (99%)	13 (1%)	73	85

All (13) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	76	LEU
1	A	177	ASN
1	A	179	THR
1	A	225	ARG
1	A	668	THR
1	A	721	HIS
1	A	755	PRO
1	B	43	GLN
1	B	318	CYS
1	B	359	LYS
1	B	469	ILE
1	B	668	THR
1	B	676	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	HIS
1	A	453	ASN
1	B	212	GLN
1	B	453	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	PNS	A	801	1	1,4,21	0.95	0	0,4,29	-	-

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	801	1	-	0/0/2/27	-

There are no bond length outliers.

There are no bond angle outliers.

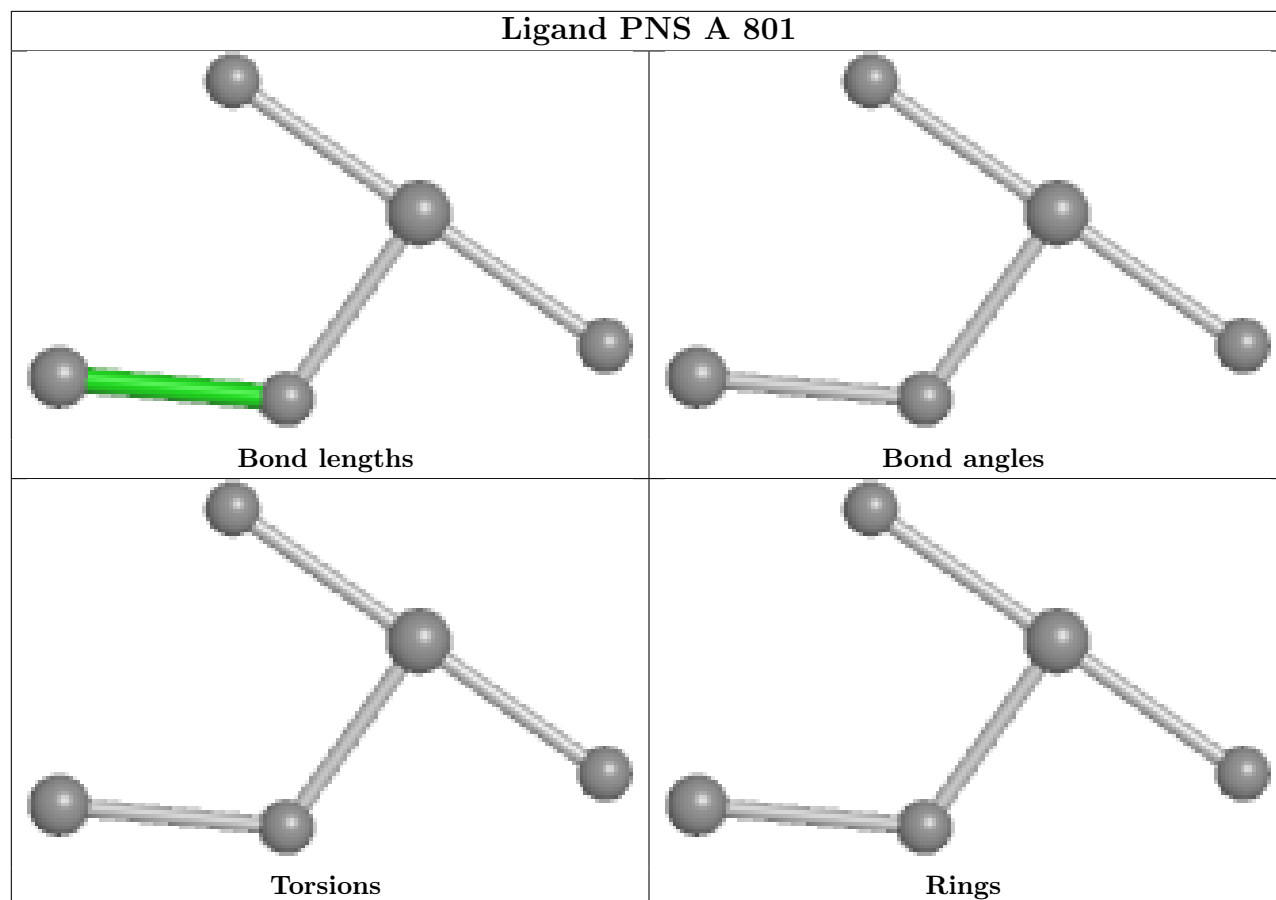
There are no chirality outliers.

There are no torsion outliers.

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, 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	759/776 (97%)	0.52	74 (9%) <b>7</b> <b>7</b>	184, 263, 353, 471	0
1	B	681/776 (87%)	0.38	64 (9%) <b>8</b> <b>7</b>	171, 236, 336, 450	0
All	All	1440/1552 (92%)	0.45	138 (9%) <b>8</b> <b>7</b>	171, 252, 347, 471	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	744	LEU	8.7
1	B	656	PRO	7.7
1	B	681	VAL	7.4
1	A	21	LEU	6.9
1	A	5	LEU	6.6
1	A	41	ASN	6.2
1	A	17	VAL	6.2
1	A	48	ILE	6.1
1	B	594	ARG	6.1
1	A	617	ALA	5.8
1	B	590	ILE	5.7
1	A	745	SER	5.5
1	B	680	ASP	5.3
1	B	615	VAL	5.3
1	B	6	PHE	4.7
1	B	665	PHE	4.6
1	A	673	VAL	4.6
1	A	642	LEU	4.5
1	B	630	TYR	4.4
1	A	628	VAL	4.3
1	B	655	ILE	4.3
1	B	659	PHE	4.3
1	A	659	PHE	4.3
1	A	746	LEU	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	750	GLN	4.1
1	A	751	LEU	4.0
1	B	658	TYR	4.0
1	A	681	VAL	3.9
1	A	69	ILE	3.9
1	B	30	ILE	3.9
1	A	615	VAL	3.9
1	A	629	GLY	3.8
1	A	616	LEU	3.8
1	A	42	LEU	3.8
1	A	658	TYR	3.7
1	A	541	GLY	3.7
1	A	554	ILE	3.7
1	A	514	LEU	3.7
1	A	722	PHE	3.7
1	A	328	SER	3.7
1	A	665	PHE	3.7
1	A	764	LEU	3.6
1	B	352	SER	3.6
1	B	41	ASN	3.6
1	A	141	PHE	3.6
1	A	463	GLY	3.5
1	A	765	THR	3.5
1	A	45	ILE	3.5
1	A	621	ALA	3.4
1	B	625	LYS	3.4
1	B	676	ARG	3.4
1	B	595	ILE	3.4
1	B	627	LEU	3.3
1	A	700	GLU	3.3
1	A	513	ILE	3.3
1	B	7	LEU	3.3
1	B	626	TYR	3.3
1	B	5	LEU	3.2
1	B	642	LEU	3.2
1	A	4	ILE	3.2
1	B	629	GLY	3.2
1	B	42	LEU	3.2
1	B	648	ASN	3.2
1	A	27	GLU	3.1
1	A	630	TYR	3.1
1	B	613	THR	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	628	VAL	3.0
1	B	604	LEU	3.0
1	B	31	CYS	3.0
1	B	657	THR	3.0
1	B	654	MET	3.0
1	B	90	VAL	3.0
1	A	502	ILE	3.0
1	B	28	VAL	3.0
1	B	49	VAL	2.9
1	A	525	ILE	2.9
1	A	579	GLU	2.9
1	B	675	ARG	2.9
1	A	716	MET	2.9
1	B	599	GLU	2.8
1	A	49	VAL	2.8
1	B	637	ILE	2.8
1	A	474	THR	2.8
1	A	77	LEU	2.8
1	A	29	VAL	2.7
1	B	617	ALA	2.7
1	A	760	LEU	2.7
1	B	469	ILE	2.7
1	B	669	ALA	2.6
1	A	563	MET	2.6
1	A	627	LEU	2.6
1	B	616	LEU	2.6
1	B	197	GLY	2.5
1	A	709	HIS	2.5
1	B	649	ASP	2.5
1	B	466	LEU	2.5
1	B	678	LEU	2.5
1	A	599	GLU	2.4
1	A	178	MET	2.4
1	A	190	LEU	2.4
1	A	283	ILE	2.4
1	A	572	PHE	2.4
1	A	70	ILE	2.4
1	B	91	TRP	2.4
1	B	100	ILE	2.4
1	A	6	PHE	2.4
1	B	653	TYR	2.4
1	A	226	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	448	PHE	2.4
1	B	196	ARG	2.3
1	A	683	ALA	2.3
1	A	710	VAL	2.3
1	B	87	PHE	2.3
1	A	321	ILE	2.3
1	B	610	ILE	2.3
1	A	323	VAL	2.3
1	B	77	LEU	2.3
1	B	120	PHE	2.3
1	A	654	MET	2.3
1	A	145	TRP	2.2
1	A	91	TRP	2.2
1	A	656	PRO	2.2
1	B	4	ILE	2.2
1	A	712	GLY	2.2
1	B	609	LEU	2.2
1	A	473	GLY	2.2
1	B	413	HIS	2.2
1	B	683	ALA	2.2
1	A	18	VAL	2.1
1	B	48	ILE	2.1
1	A	448	PHE	2.1
1	B	641	GLU	2.1
1	A	303	ILE	2.1
1	B	390	TYR	2.1
1	B	158	GLN	2.1
1	B	57	LEU	2.1
1	A	362	MET	2.1
1	A	120	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](#)

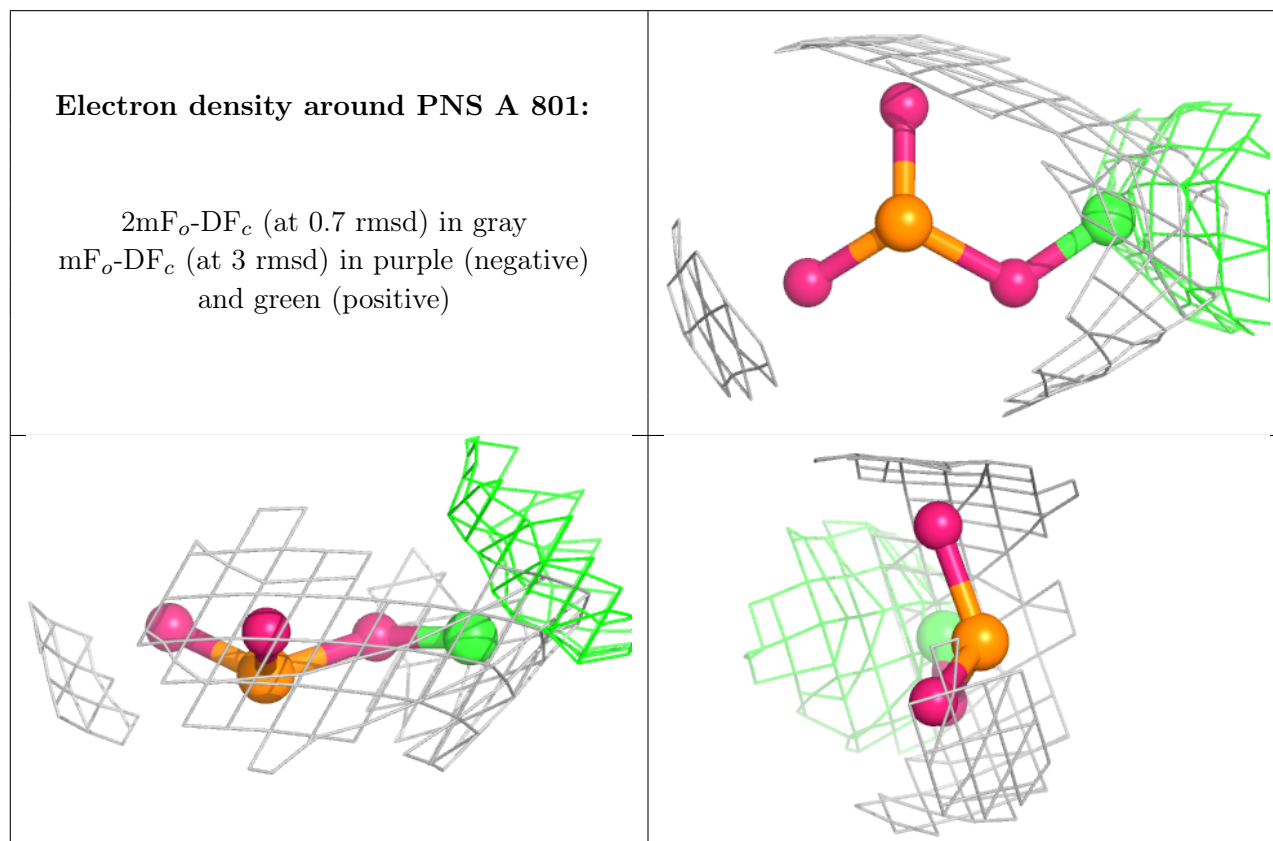
There are no monosaccharides in this entry.

## 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
2	PNS	A	801	5/22	0.62	0.66	266,268,288,306	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 [i](#)

There are no such residues in this entry.