



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:58 AM UTC

PDB ID : 6MFY / pdb_00006mfy
Title : Crystal structure of a 5-domain construct of LgrA in the substrate donation state
Authors : Reimer, J.M.; Eivaskhani, M.; Harb, I.; Schmeing, T.M.
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 types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

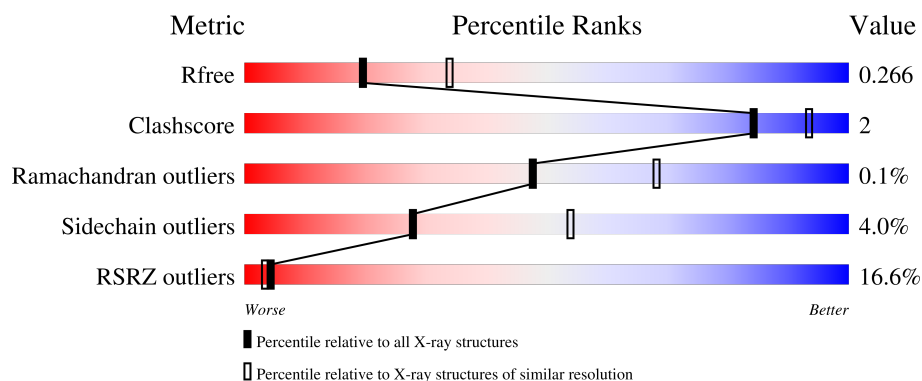
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of 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	15% 82% 9% 8%

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.

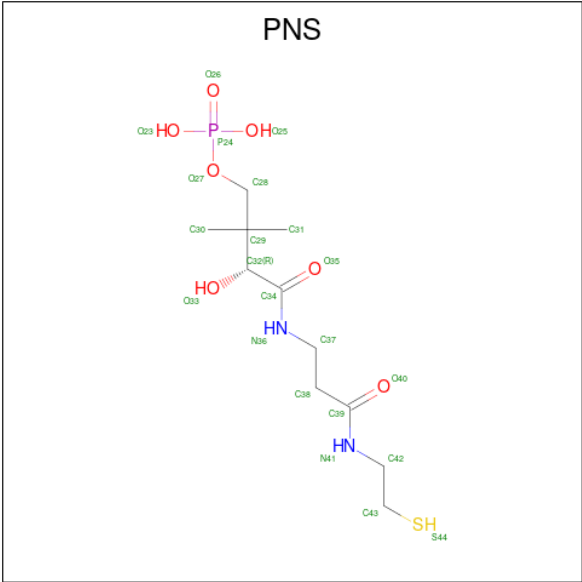
- Molecule 1 is a protein called Linear gramicidin synthase subunit A.

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:

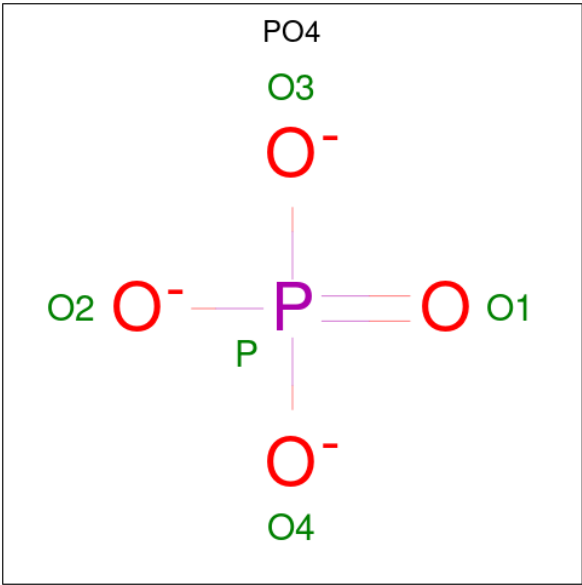
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q70LM7
A	0	ALA	-	expression tag	UNP Q70LM7
A	1	MET	-	expression tag	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	1718	ALA	-	expression tag	UNP Q70LM7
A	1719	ALA	-	expression tag	UNP Q70LM7
A	1720	ALA	-	expression tag	UNP 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 (CCD ID: 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 (CCD ID: 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		

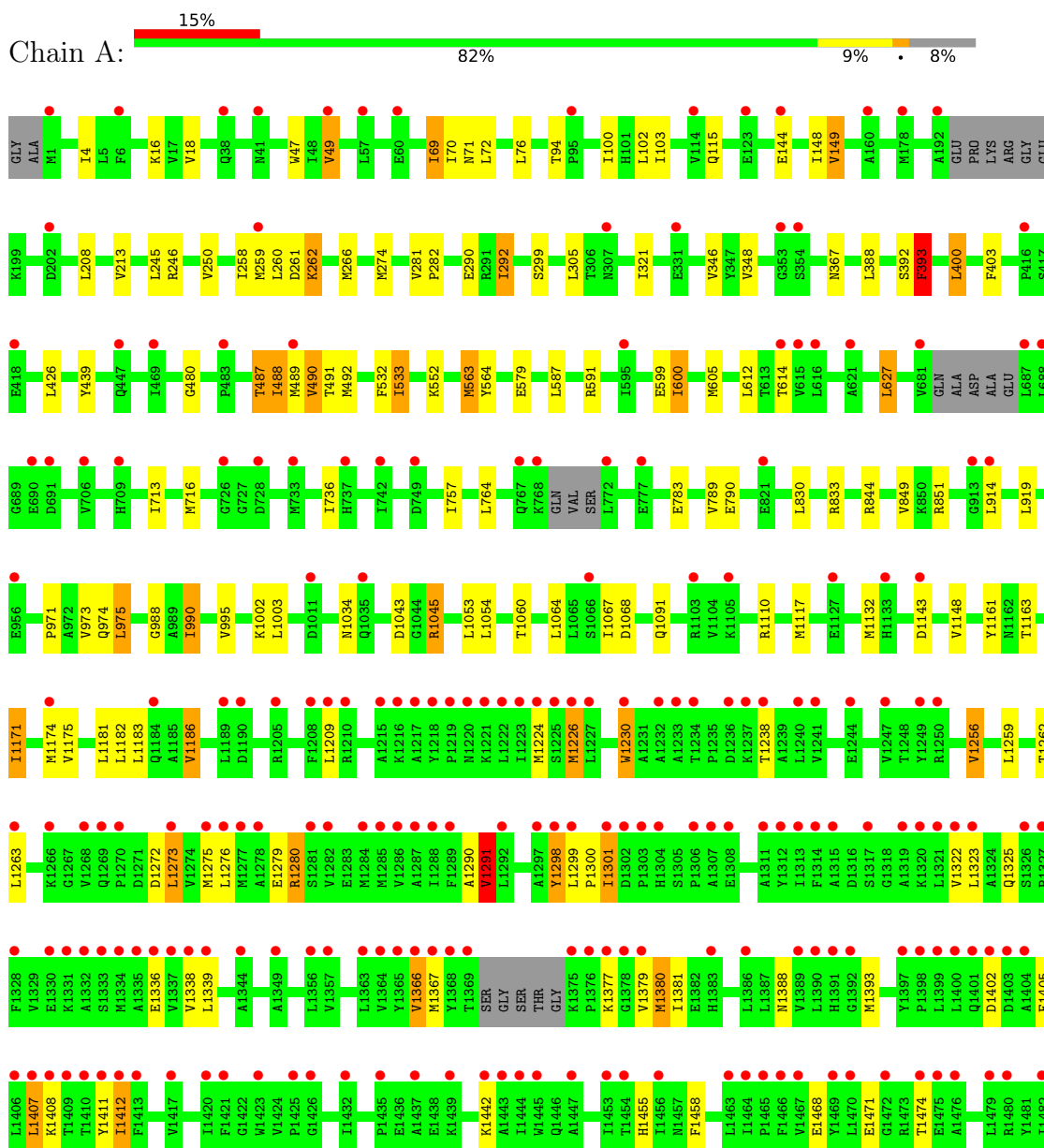
- Molecule 4 is water.

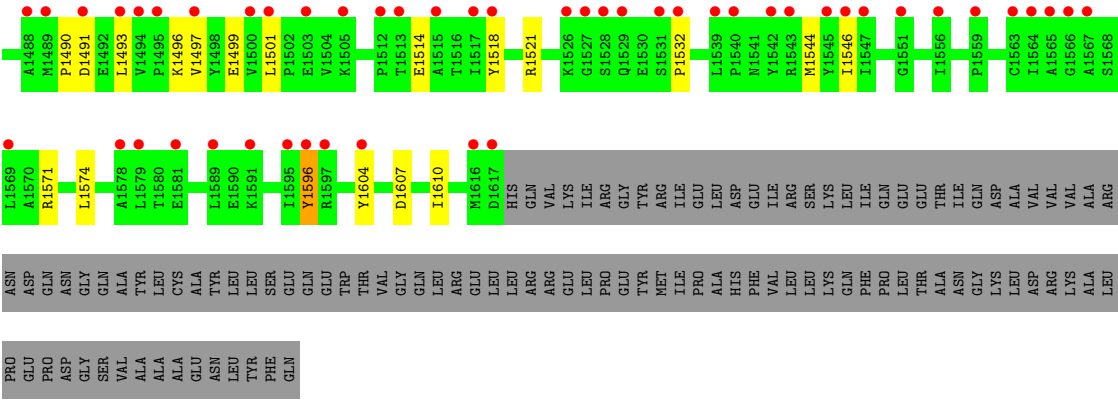
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	0
			100	100		

3 Residue-property plots

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 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 85.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (85.77-2.50) 99.5 (85.77-2.50)	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 0.238 , 0.266	Depositor DCC
R_{free} test set	3793 reflections (4.98%)	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)	0.33 , 38.4	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	0.93	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: PO4, 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	0.68	61/12976 (0.5%)	0.80	39/17619 (0.2%)

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	VAL	C-O	-9.40	1.15	1.24
1	A	100	ILE	C-O	-8.44	1.14	1.24
1	A	1148	VAL	C-O	-8.44	1.15	1.24
1	A	148	ILE	C-N	8.36	1.44	1.33
1	A	490	VAL	C-O	-8.32	1.15	1.24
1	A	1003	LEU	C-O	-8.26	1.14	1.24
1	A	321	ILE	C-O	-8.21	1.14	1.24
1	A	392	SER	C-N	-8.14	1.23	1.34
1	A	919	LEU	C-O	-7.94	1.15	1.24
1	A	533	ILE	C-O	-7.92	1.15	1.24
1	A	1322	VAL	C-N	7.91	1.44	1.33
1	A	627	LEU	C-O	-7.86	1.14	1.24
1	A	69	ILE	C-O	-7.69	1.15	1.24
1	A	789	VAL	C-N	-7.67	1.24	1.33
1	A	599	GLU	C-N	-7.65	1.25	1.33
1	A	208	LEU	C-O	-7.61	1.15	1.24
1	A	245	LEU	C-O	-7.49	1.15	1.24
1	A	973	VAL	C-O	-7.41	1.15	1.24
1	A	70	ILE	C-O	-7.25	1.15	1.24
1	A	426	LEU	C-O	-7.20	1.15	1.24
1	A	260	LEU	C-O	-7.02	1.15	1.23
1	A	1054	LEU	C-O	-6.86	1.15	1.23
1	A	1053	LEU	C-O	-6.75	1.15	1.24
1	A	439	TYR	C-O	-6.75	1.16	1.24
1	A	388	LEU	C-O	-6.64	1.15	1.24
1	A	305	LEU	C-O	-6.59	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	587	LEU	C-O	-6.54	1.15	1.23
1	A	1181	LEU	C-O	-6.52	1.16	1.24
1	A	103	ILE	C-O	-6.52	1.17	1.24
1	A	830	LEU	C-O	-6.46	1.16	1.24
1	A	491	THR	C-O	-6.43	1.15	1.23
1	A	833	ARG	C-O	-6.33	1.15	1.24
1	A	18	VAL	C-O	-6.31	1.17	1.24
1	A	600	ILE	C-O	-6.28	1.15	1.24
1	A	1067	ILE	C-O	-6.18	1.17	1.23
1	A	990	ILE	C-N	6.04	1.42	1.33
1	A	563	MET	C-N	6.04	1.41	1.33
1	A	102	LEU	C-O	-5.92	1.16	1.24
1	A	783	GLU	C-O	-5.88	1.16	1.23
1	A	1091	GLN	C-O	-5.85	1.16	1.24
1	A	1132	MET	C-O	-5.83	1.16	1.24
1	A	851	ARG	C-O	-5.81	1.16	1.24
1	A	1034	ASN	C-O	-5.80	1.17	1.24
1	A	1300	PRO	C-O	-5.74	1.17	1.23
1	A	1325	GLN	C-O	-5.71	1.16	1.23
1	A	1043	ASP	CG-OD2	-5.70	1.14	1.25
1	A	736	ILE	C-O	-5.64	1.17	1.24
1	A	1068	ASP	C-O	-5.63	1.16	1.23
1	A	1226	MET	C-N	5.42	1.41	1.33
1	A	246	ARG	C-O	-5.33	1.17	1.24
1	A	757	ILE	C-O	-5.32	1.17	1.24
1	A	1110	ARG	C-O	-5.30	1.17	1.23
1	A	1388	ASN	C-O	-5.29	1.18	1.24
1	A	1299	LEU	C-O	-5.27	1.18	1.24
1	A	1183	LEU	C-O	-5.25	1.17	1.24
1	A	1043	ASP	C-O	-5.23	1.17	1.24
1	A	1045	ARG	C-O	-5.23	1.15	1.23
1	A	971	PRO	C-O	-5.19	1.18	1.23
1	A	1490	PRO	C-O	-5.16	1.17	1.23
1	A	1186	VAL	C-O	-5.10	1.17	1.24
1	A	213	VAL	C-O	-5.07	1.18	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	VAL	N-CA-CB	9.63	121.81	110.55
1	A	789	VAL	CA-C-N	9.47	132.75	120.44
1	A	789	VAL	C-N-CA	9.47	132.75	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1174	MET	CA-C-N	8.96	131.85	120.56
1	A	1174	MET	C-N-CA	8.96	131.85	120.56
1	A	392	SER	CA-C-N	8.64	133.00	120.38
1	A	392	SER	C-N-CA	8.64	133.00	120.38
1	A	393	PHE	CA-CB-CG	8.18	121.97	113.80
1	A	995	VAL	N-CA-C	-7.37	100.09	109.30
1	A	1388	ASN	CA-CB-CG	-7.06	105.54	112.60
1	A	393	PHE	CB-CA-C	7.02	124.08	110.46
1	A	262	LYS	CB-CA-C	6.83	120.00	110.16
1	A	246	ARG	N-CA-C	-6.56	104.21	111.36
1	A	1380	MET	CA-C-N	-6.37	114.08	122.94
1	A	1380	MET	C-N-CA	-6.37	114.08	122.94
1	A	1596	TYR	CA-C-O	-6.31	113.61	120.36
1	A	262	LYS	N-CA-C	-6.30	100.57	109.96
1	A	1291	VAL	N-CA-C	-6.28	104.39	110.42
1	A	400	LEU	N-CA-C	-6.16	104.19	111.03
1	A	1379	VAL	CA-C-N	6.10	131.17	121.66
1	A	1379	VAL	C-N-CA	6.10	131.17	121.66
1	A	1412	ILE	N-CA-C	-6.04	106.54	111.91
1	A	995	VAL	N-CA-CB	5.94	117.62	110.31
1	A	321	ILE	N-CA-CB	-5.76	105.17	112.15
1	A	1262	THR	CA-C-N	5.62	127.74	120.44
1	A	1262	THR	C-N-CA	5.62	127.74	120.44
1	A	260	LEU	CA-C-O	-5.59	115.08	121.40
1	A	1298	TYR	CB-CA-C	5.51	119.12	110.19
1	A	790	GLU	N-CA-C	-5.49	105.20	111.07
1	A	367	ASN	N-CA-C	-5.40	105.31	111.14
1	A	1280	ARG	CB-CA-C	5.38	121.14	110.42
1	A	71	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	1045	ARG	N-CA-C	-5.29	101.61	109.11
1	A	1405	PHE	CA-C-N	5.28	129.90	122.09
1	A	1405	PHE	C-N-CA	5.28	129.90	122.09
1	A	144	GLU	CB-CA-C	5.27	119.62	110.72
1	A	1497	VAL	CA-C-N	5.13	127.11	120.44
1	A	1497	VAL	C-N-CA	5.13	127.11	120.44
1	A	1299	LEU	CA-C-O	-5.09	115.14	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12694	0	12564	58	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	12585	58	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 (58) 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:489:MET:SD	1:A:492:MET:HE1	2.15	0.87
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:1275:MET:HE2	1:A:1301:ILE:HD11	1.70	0.72
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:400:LEU:HD23	1:A:400:LEU:C	2.26	0.61
1:A:605:MET:HE2	1:A:612:LEU:HA	1.83	0.61
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	2.03	0.58
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:1393:MET:HE2	1:A:1518:TYR:CE2	2.41	0.55
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:716:MET:HA	1:A:716:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:LYS:HB3	1:A:564:TYR:CE1	2.43	0.53
1:A:914:LEU:HB3	1:A:1045:ARG:NH2	2.24	0.52
1:A:1532:PRO:O	1:A:1532:PRO:HG2	2.10	0.52
1:A:282:PRO:HD2	1:A:348:VAL:O	2.11	0.51
1:A:261:ASP:C	1:A:266:MET:HE3	2.36	0.51
1:A:259:MET:HE1	1:A:292:ILE:HG23	1.93	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:1279:GLU:O	1:A:1280:ARG:C	2.55	0.50
1:A:1514:GLU:HG2	1:A:1596:TYR:CE1	2.48	0.49
1:A:274:MET:HE2	1:A:346:VAL:HG22	1.95	0.48
1:A:614:THR:O	1:A:614:THR:HG22	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:400:LEU:HD12	1:A:488:ILE:HG21	1.96	0.47
1:A:1367:MET:HE1	1:A:1412:ILE:O	2.14	0.47
1:A:1060:THR:HG23	1:A:1117:MET:HE1	1.97	0.46
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: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:76:LEU:HD12	1:A:115:GLN:CD	2.42	0.44
1:A:1544:MET:SD	1:A:1610:ILE:HD12	2.57	0.44
1:A:274:MET:HE2	1:A:346:VAL:CG2	2.48	0.44
1:A:600:ILE:CD1	1:A:627:LEU:HD13	2.47	0.44
1:A:1182:LEU:C	1:A:1182:LEU:HD23	2.42	0.44
1:A:274:MET:HE1	1:A:403:PHE:CE1	2.54	0.43
1:A:1256:VAL:HG13	1:A:1290:ALA:HB2	2.01	0.43
1:A:1259:LEU:HD23	1:A:1259:LEU:C	2.41	0.43
1:A:1272:ASP:C	1:A:1272:ASP:OD1	2.62	0.42
1:A:532:PHE:CD2	1:A:563:MET:HE3	2.55	0.42
1:A:974:GLN:C	1:A:975:LEU:HD23	2.45	0.41
1:A:988:GLY:C	1:A:1163:THR:HG23	2.45	0.40
1:A:1367:MET:HE1	1:A:1412:ILE:C	2.46	0.40
1:A:1275:MET:HE2	1:A:1301:ILE:CD1	2.45	0.40

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%)	48 68

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%)	1304 (96%)	55 (4%)	28 54

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	49	VAL
1	A	69	ILE
1	A	94	THR
1	A	149	VAL
1	A	290	GLU
1	A	292	ILE
1	A	393	PHE
1	A	579	GLU

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Mol	Chain	Res	Type
1	A	591	ARG
1	A	713	ILE
1	A	764	LEU
1	A	844	ARG
1	A	849	VAL
1	A	975	LEU
1	A	990	ILE
1	A	1002	LYS
1	A	1064	LEU
1	A	1143	ASP
1	A	1171	ILE
1	A	1175	VAL
1	A	1186	VAL
1	A	1209	LEU
1	A	1224	MET
1	A	1226	MET
1	A	1230	TRP
1	A	1238	THR
1	A	1256	VAL
1	A	1273	LEU
1	A	1276	LEU
1	A	1291	VAL
1	A	1301	ILE
1	A	1336	GLU
1	A	1338	VAL
1	A	1366	VAL
1	A	1377	LYS
1	A	1381	ILE
1	A	1402	ASP
1	A	1407	LEU
1	A	1408	LYS
1	A	1411	TYR
1	A	1442	LYS
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	1499	GLU

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Mol	Chain	Res	Type
1	A	1501	LEU
1	A	1521	ARG
1	A	1574	LEU
1	A	1607	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	558	GLN
1	A	781	GLN
1	A	871	GLN
1	A	1079	GLN
1	A	1133	HIS
1	A	1258	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1810	-	4,4,4	0.93	0	6,6,6	0.47	0
3	PO4	A	1802	-	4,4,4	0.98	0	6,6,6	0.46	0
3	PO4	A	1808	-	4,4,4	0.90	0	6,6,6	0.47	0
3	PO4	A	1806	-	4,4,4	0.95	0	6,6,6	0.45	0
3	PO4	A	1804	-	4,4,4	0.93	0	6,6,6	0.54	0
3	PO4	A	1805	-	4,4,4	0.93	0	6,6,6	0.43	0
2	PNS	A	1801	1	14,20,21	2.20	4 (28%)	18,26,29	1.43	4 (22%)
3	PO4	A	1803	-	4,4,4	0.96	0	6,6,6	0.46	0
3	PO4	A	1811	-	4,4,4	0.92	0	6,6,6	0.48	0
3	PO4	A	1807	-	4,4,4	0.96	0	6,6,6	0.46	0
3	PO4	A	1809	-	4,4,4	0.95	0	6,6,6	0.44	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
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	5.22	1.45	1.33
2	A	1801	PNS	C39-N41	5.14	1.45	1.33
2	A	1801	PNS	O35-C34	-2.28	1.19	1.23
2	A	1801	PNS	O40-C39	-2.14	1.19	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1801	PNS	C38-C39-N41	2.72	121.29	116.34
2	A	1801	PNS	C37-C38-C39	-2.58	108.10	112.39
2	A	1801	PNS	C42-N41-C39	-2.40	118.36	122.82
2	A	1801	PNS	C32-C34-N36	2.12	120.51	116.48

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

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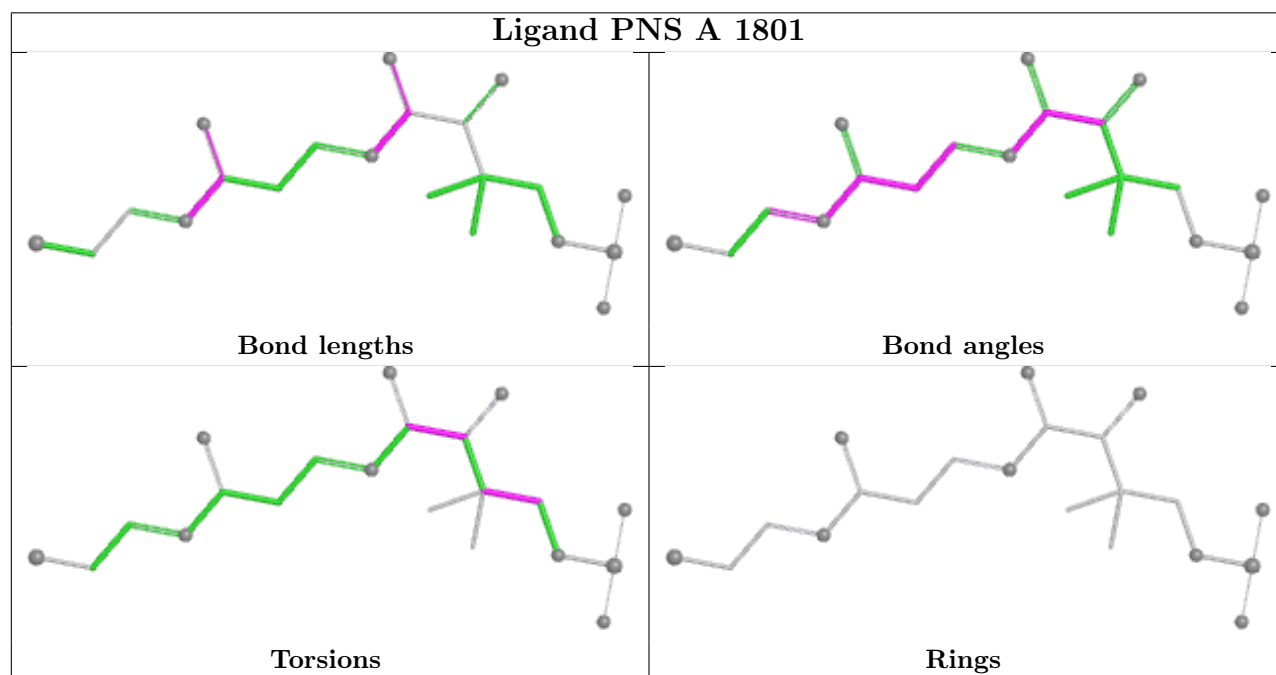
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Mol	Chain	Res	Type	Atoms
2	A	1801	PNS	O33-C32-C34-N36
2	A	1801	PNS	O27-C28-C29-C30

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 ⓘ

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%)	0.93	266 (16%) 4 3	37, 61, 153, 184	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1143	ASP	7.0
1	A	687	LEU	5.7
1	A	1285	MET	5.7
1	A	1470	LEU	5.2
1	A	1369	THR	5.1
1	A	1238	THR	5.0
1	A	1363	LEU	4.7
1	A	772	LEU	4.6
1	A	614	THR	4.5
1	A	1307	ALA	4.4
1	A	1357	VAL	4.4
1	A	1488	ALA	4.3
1	A	1282	VAL	4.3
1	A	1298	TYR	4.3
1	A	1517	ILE	4.1
1	A	726	GLY	4.0
1	A	1376	PRO	4.0
1	A	1475	GLU	4.0
1	A	1539	LEU	4.0
1	A	1313	ILE	3.9
1	A	1617	ASP	3.9
1	A	1474	THR	3.9
1	A	1268	VAL	3.9
1	A	1319	ALA	3.8
1	A	1410	THR	3.8
1	A	1337	VAL	3.8
1	A	1379	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	144	GLU	3.8
1	A	1299	LEU	3.8
1	A	1493	LEU	3.8
1	A	1216	LYS	3.7
1	A	1447	ALA	3.7
1	A	416	PRO	3.7
1	A	1454	THR	3.7
1	A	1390	LEU	3.7
1	A	1567	ALA	3.6
1	A	1269	GLN	3.6
1	A	1230	TRP	3.6
1	A	1444	ILE	3.6
1	A	1453	ILE	3.6
1	A	1306	PRO	3.6
1	A	202	ASP	3.6
1	A	1276	LEU	3.6
1	A	1421	PHE	3.6
1	A	1366	VAL	3.5
1	A	1497	VAL	3.5
1	A	1189	LEU	3.5
1	A	1403	ASP	3.5
1	A	1518	TYR	3.5
1	A	1344	ALA	3.5
1	A	1392	GLY	3.5
1	A	1011	ASP	3.5
1	A	1413	PHE	3.5
1	A	1399	LEU	3.4
1	A	1368	TYR	3.4
1	A	1466	PHE	3.4
1	A	1423	TRP	3.3
1	A	1391	HIS	3.3
1	A	1301	ILE	3.3
1	A	1323	LEU	3.3
1	A	1311	ALA	3.3
1	A	1221	LYS	3.3
1	A	688	LEU	3.3
1	A	1209	LEU	3.3
1	A	1286	VAL	3.3
1	A	1233	ALA	3.3
1	A	1320	LYS	3.3
1	A	1241	VAL	3.2
1	A	1565	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1225	SER	3.2
1	A	1463	LEU	3.2
1	A	353	GLY	3.2
1	A	1417	VAL	3.2
1	A	1219	PRO	3.1
1	A	1479	LEU	3.1
1	A	307	ASN	3.1
1	A	1331	LYS	3.1
1	A	1336	GLU	3.1
1	A	1327	PRO	3.1
1	A	1328	PHE	3.1
1	A	1220	ASN	3.1
1	A	1398	PRO	3.1
1	A	1409	THR	3.0
1	A	1332	ALA	3.0
1	A	913	GLY	3.0
1	A	1527	GLY	3.0
1	A	1335	ALA	3.0
1	A	1411	TYR	3.0
1	A	1263	LEU	3.0
1	A	1266	LYS	3.0
1	A	1556	ILE	3.0
1	A	1589	LEU	3.0
1	A	1439	LYS	3.0
1	A	1174	MET	3.0
1	A	1402	ASP	3.0
1	A	1529	GLN	3.0
1	A	1289	PHE	2.9
1	A	1566	GLY	2.9
1	A	595	ILE	2.9
1	A	469	ILE	2.9
1	A	1512	PRO	2.9
1	A	1532	PRO	2.9
1	A	1217	ALA	2.9
1	A	1472	GLY	2.9
1	A	737	HIS	2.8
1	A	1464	ILE	2.8
1	A	1540	PRO	2.8
1	A	1356	LEU	2.8
1	A	1249	TYR	2.8
1	A	1482	ILE	2.8
1	A	615	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	160	ALA	2.8
1	A	1443	ALA	2.8
1	A	1334	MET	2.8
1	A	777	GLU	2.8
1	A	1564	ILE	2.7
1	A	1227	LEU	2.7
1	A	1275	MET	2.7
1	A	1386	LEU	2.7
1	A	821	GLU	2.7
1	A	38	GLN	2.7
1	A	1066	SER	2.7
1	A	1339	LEU	2.7
1	A	1035	GLN	2.7
1	A	1270	PRO	2.7
1	A	1494	VAL	2.7
1	A	1287	ALA	2.7
1	A	1503	GLU	2.7
1	A	1515	ALA	2.7
1	A	1304	HIS	2.7
1	A	1314	PHE	2.6
1	A	1469	TYR	2.6
1	A	1375	LYS	2.6
1	A	57	LEU	2.6
1	A	1467	VAL	2.6
1	A	1349	ALA	2.6
1	A	1237	LYS	2.6
1	A	1365	TYR	2.6
1	A	749	ASP	2.5
1	A	1412	ILE	2.5
1	A	1222	LEU	2.5
1	A	1500	VAL	2.5
1	A	192	ALA	2.5
1	A	768	LYS	2.5
1	A	1495	PRO	2.5
1	A	1273	LEU	2.5
1	A	1404	ALA	2.5
1	A	259	MET	2.5
1	A	1288	ILE	2.5
1	A	1321	LEU	2.5
1	A	1408	LYS	2.5
1	A	1338	VAL	2.5
1	A	1383	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	418	GLU	2.5
1	A	1406	LEU	2.5
1	A	1501	LEU	2.5
1	A	1437	ALA	2.5
1	A	354	SER	2.5
1	A	1326	SER	2.5
1	A	1333	SER	2.5
1	A	728	ASP	2.4
1	A	1545	TYR	2.4
1	A	1579	LEU	2.4
1	A	767	GLN	2.4
1	A	1284	MET	2.4
1	A	1317	SER	2.4
1	A	1407	LEU	2.4
1	A	1596	TYR	2.4
1	A	1476	ALA	2.4
1	A	691	ASP	2.4
1	A	1456	ILE	2.4
1	A	1397	TYR	2.4
1	A	621	ALA	2.4
1	A	1445	TRP	2.4
1	A	1442	LYS	2.4
1	A	1292	LEU	2.4
1	A	1480	ARG	2.4
1	A	1569	LEU	2.4
1	A	1389	VAL	2.4
1	A	1435	PRO	2.3
1	A	483	PRO	2.3
1	A	1210	ARG	2.3
1	A	1531	SER	2.3
1	A	1312	TYR	2.3
1	A	1528	SER	2.3
1	A	1595	ILE	2.3
1	A	1367	MET	2.3
1	A	1616	MET	2.3
1	A	1322	VAL	2.3
1	A	1364	VAL	2.3
1	A	1542	TYR	2.3
1	A	41	ASN	2.3
1	A	1278	ALA	2.3
1	A	1303	PRO	2.3
1	A	1420	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1432	ILE	2.3
1	A	1226	MET	2.3
1	A	1105	LYS	2.3
1	A	706	VAL	2.3
1	A	1103	ARG	2.3
1	A	1133	HIS	2.2
1	A	1302	ASP	2.2
1	A	1491	ASP	2.2
1	A	1244	GLU	2.2
1	A	1581	GLU	2.2
1	A	681	VAL	2.2
1	A	1401	GLN	2.2
1	A	489	MET	2.2
1	A	1378	GLY	2.2
1	A	742	ILE	2.2
1	A	1547	ILE	2.2
1	A	956	GLU	2.2
1	A	1597	ARG	2.2
1	A	114	VAL	2.2
1	A	1297	ALA	2.2
1	A	1505	LYS	2.2
1	A	178	MET	2.2
1	A	1234	THR	2.2
1	A	1223	ILE	2.2
1	A	1190	ASP	2.2
1	A	123	GLU	2.2
1	A	1330	GLU	2.2
1	A	1377	LYS	2.2
1	A	1526	LYS	2.2
1	A	1277	MET	2.2
1	A	690	GLU	2.2
1	A	1184	GLN	2.1
1	A	616	LEU	2.1
1	A	1563	CYS	2.1
1	A	1205	ARG	2.1
1	A	1308	GLU	2.1
1	A	1281	SER	2.1
1	A	49	VAL	2.1
1	A	1247	VAL	2.1
1	A	1315	ALA	2.1
1	A	1240	LEU	2.1
1	A	1546	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1604	TYR	2.1
1	A	95	PRO	2.1
1	A	1465	PRO	2.1
1	A	6	PHE	2.1
1	A	1489	MET	2.1
1	A	1400	LEU	2.1
1	A	1543	ARG	2.1
1	A	60	GLU	2.1
1	A	1425	PRO	2.1
1	A	709	HIS	2.1
1	A	447	GLN	2.1
1	A	914	LEU	2.1
1	A	1250	ARG	2.1
1	A	1426	GLY	2.1
1	A	331	GLU	2.1
1	A	1127	GLU	2.1
1	A	1218	TYR	2.1
1	A	1236	ASP	2.1
1	A	1559	PRO	2.1
1	A	1551	GLY	2.0
1	A	1	MET	2.0
1	A	1208	PHE	2.0
1	A	1215	ALA	2.0
1	A	1232	ALA	2.0
1	A	1578	ALA	2.0
1	A	1591	LYS	2.0
1	A	1513	THR	2.0
1	A	733	MET	2.0
1	A	1224	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

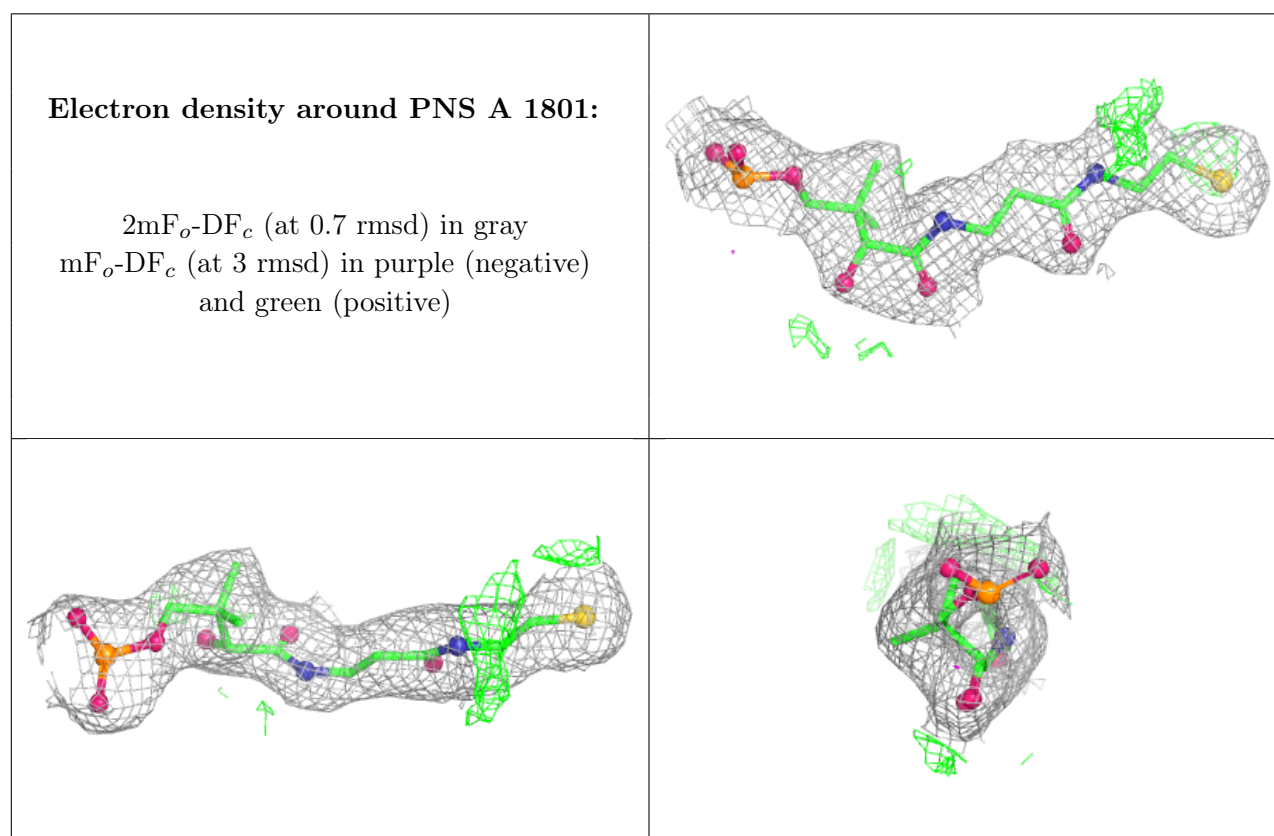
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	PO4	A	1810	5/5	0.37	0.20	80,86,88,89	0
3	PO4	A	1808	5/5	0.49	0.24	82,83,85,85	0
3	PO4	A	1805	5/5	0.50	0.17	82,83,85,87	0
3	PO4	A	1809	5/5	0.53	0.16	83,85,87,88	0
3	PO4	A	1806	5/5	0.56	0.17	82,82,83,83	0
3	PO4	A	1807	5/5	0.58	0.14	80,81,83,89	0
3	PO4	A	1811	5/5	0.71	0.26	80,80,85,86	0
3	PO4	A	1804	5/5	0.73	0.18	82,83,85,89	0
3	PO4	A	1803	5/5	0.76	0.19	80,81,83,83	0
2	PNS	A	1801	21/22	0.93	0.10	45,48,53,56	0
3	PO4	A	1802	5/5	0.96	0.07	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 [i](#)

There are no such residues in this entry.