



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:30 PM UTC

PDB ID : 7X0F / pdb_00007x0f
Title : Structure of Pseudomonas NRPS protein, AmbB-TC bound to Ppant
Authors : ChuYuanKee, M.; Bharath, S.R.; Song, H.
Deposited on : 2022-02-22
Resolution : 2.20 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

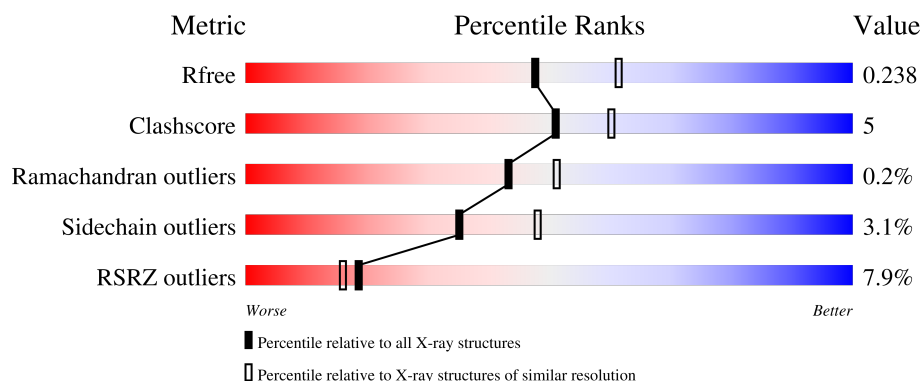
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	523	14% 75% 10% • 15%
1	B	523	5% 76% 9% • 14%
1	C	523	3% 80% 8% 12%
1	D	523	6% 79% 7% 15%

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	B	1301	-	-	X	-

2 Entry composition [i](#)

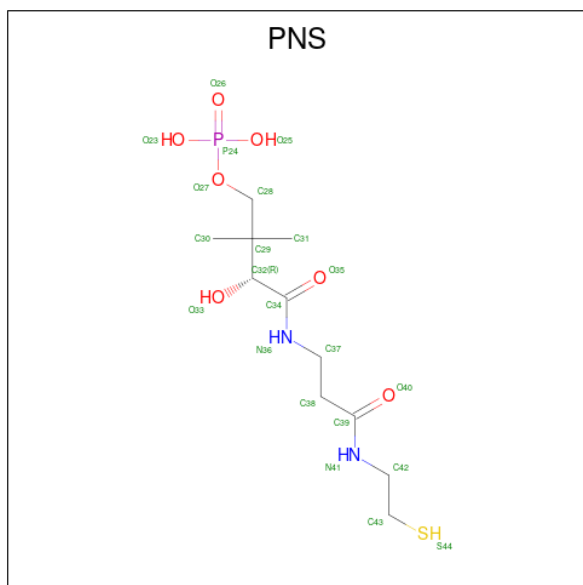
There are 3 unique types of molecules in this entry. The entry contains 14566 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AMB antimetabolite synthase AmbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3424	2159	652	608	5			
1	B	452	Total	C	N	O	S	0	0	0
			3454	2174	660	615	5			
1	C	458	Total	C	N	O	S	0	0	0
			3510	2210	670	625	5			
1	D	447	Total	C	N	O	S	0	0	0
			3425	2160	655	605	5			

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS) (labeled as "Ligand of Interest" by depositor).



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

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

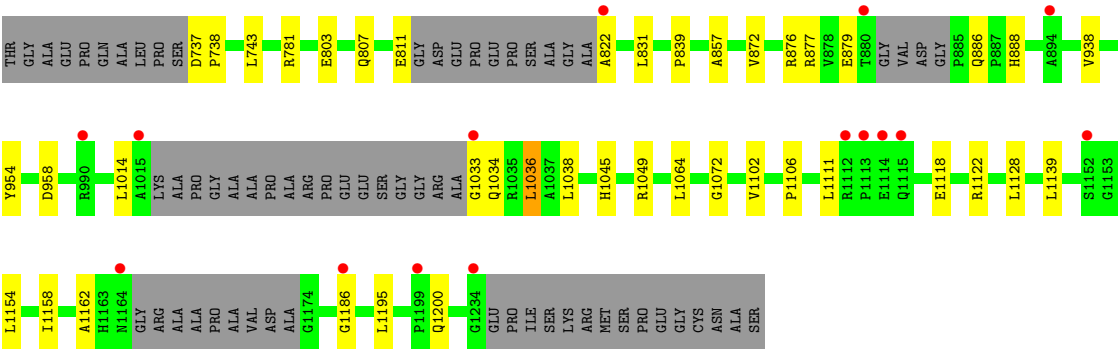
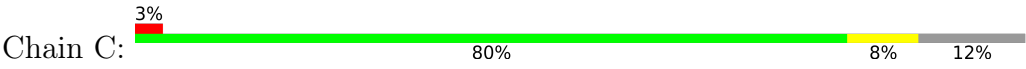
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	159	Total	O	0	0
			159	159		
3	B	187	Total	O	0	0
			187	187		
3	C	180	Total	O	0	0
			180	180		
3	D	143	Total	O	0	0
			143	143		

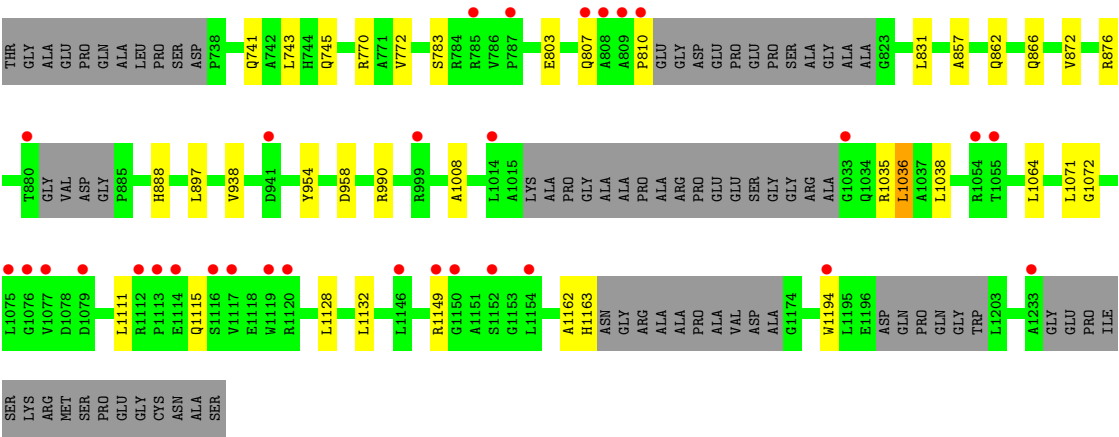
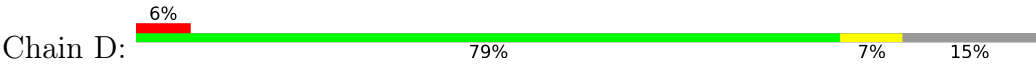
i

- Molecule 1: AMB antimetabolite synthase AmbB





• Molecule 1: AMB antimetabolite synthase AmbB



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.41Å 71.19Å 172.77Å 90.00° 109.93° 90.00°	Depositor
Resolution (Å)	49.56 – 2.20 49.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.56-2.20) 98.8 (49.56-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0261	Depositor
R, R_{free}	0.210 , 0.240 0.210 , 0.238	Depositor DCC
R_{free} test set	5662 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.4	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	0.94	EDS
Total number of atoms	14566	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

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	0.76	0/3482	0.96	0/4731
1	B	0.77	0/3512	0.99	2/4771 (0.0%)
1	C	0.78	0/3573	0.97	0/4858
1	D	0.73	0/3484	0.96	1/4733 (0.0%)
All	All	0.76	0/14051	0.97	3/19093 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	766	GLY	N-CA-C	7.46	124.64	111.73
1	D	770	ARG	CB-CG-CD	5.33	123.56	111.30
1	B	767	ASP	N-CA-CB	5.12	119.15	110.49

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	3424	0	3482	47	0
1	B	3454	0	3519	45	0
1	C	3510	0	3565	29	0
1	D	3425	0	3501	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	21	0	21	3	0
2	B	21	0	21	11	0
2	C	21	0	21	2	0
2	D	21	0	21	5	0
3	A	159	0	0	2	0
3	B	187	0	0	3	0
3	C	180	0	0	4	0
3	D	143	0	0	4	0
All	All	14566	0	14151	146	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 5.

All (146) 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:743:LEU:HD13	1:A:802:LEU:CD2	1.65	1.26
1:A:743:LEU:HD13	1:A:802:LEU:HD21	1.45	0.95
1:A:743:LEU:HD13	1:A:802:LEU:HD23	1.46	0.95
1:A:743:LEU:CD1	1:A:802:LEU:HD23	2.02	0.87
1:A:1036:LEU:HD13	1:A:1215:LEU:HD11	1.60	0.81
1:A:745:GLN:HA	1:A:748:GLN:HE21	1.43	0.81
1:A:743:LEU:CD1	1:A:802:LEU:CD2	2.52	0.80
1:A:798:PRO:O	1:A:802:LEU:HG	1.83	0.78
1:B:958:ASP:HB2	2:B:1301:PNS:H432	1.70	0.72
2:A:1301:PNS:O35	2:A:1301:PNS:H303	1.88	0.71
1:B:736:SER:O	1:B:737:ASP:C	2.36	0.69
1:A:781:ARG:O	1:A:783:SER:N	2.24	0.69
1:A:784:ARG:NH1	1:A:808:ALA:O	2.27	0.68
1:B:1174:GLY:N	3:B:1403:HOH:O	2.28	0.67
1:B:1094:MET:HA	1:B:1097:LEU:HD22	1.76	0.67
1:C:839:PRO:HG3	3:C:1408:HOH:O	1.95	0.67
1:A:1173:ALA:N	3:A:1402:HOH:O	2.31	0.64
1:B:779:ARG:HD2	1:B:785:ARG:CZ	2.28	0.63
1:B:958:ASP:CB	2:B:1301:PNS:H432	2.29	0.63
1:B:767:ASP:HB2	1:B:770:ARG:HD3	1.82	0.62
1:D:783:SER:O	1:D:810:PRO:HA	1.99	0.62
1:C:1036:LEU:HD11	1:C:1038:LEU:HD11	1.82	0.62
1:A:771:ALA:O	1:A:775:LEU:HD23	2.01	0.61
1:A:1158:ILE:CD1	1:A:1191:LEU:HB3	2.30	0.61
1:C:1034:GLN:NE2	3:C:1401:HOH:O	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:LEU:HD13	1:A:802:LEU:CG	2.29	0.60
1:B:762:TYR:HA	1:B:766:GLY:HA3	1.83	0.59
1:A:1091:ARG:NH2	1:A:1093:GLU:OE2	2.36	0.59
1:C:822:ALA:O	1:C:886:GLN:OE1	2.21	0.58
1:B:1060:PHE:CE2	2:B:1301:PNS:H311	2.39	0.58
1:A:781:ARG:CZ	1:A:781:ARG:HA	2.33	0.58
1:A:1064:LEU:C	1:A:1064:LEU:HD23	2.29	0.57
1:C:857:ALA:HB2	1:C:938:VAL:HG21	1.84	0.57
1:B:857:ALA:HB2	1:B:938:VAL:HG11	1.86	0.57
1:B:864:LEU:HD21	1:B:947:LEU:HD11	1.85	0.57
1:D:1064:LEU:C	1:D:1064:LEU:HD23	2.30	0.57
1:D:1035:ARG:HD2	3:D:1514:HOH:O	2.03	0.57
1:A:745:GLN:HA	1:A:748:GLN:NE2	2.19	0.56
1:B:1060:PHE:CD2	2:B:1301:PNS:H311	2.40	0.56
1:B:1102:VAL:CG1	2:B:1301:PNS:H431	2.35	0.56
1:D:1163:HIS:CE1	1:D:1194:TRP:CZ3	2.94	0.56
2:D:1301:PNS:H421	3:D:1495:HOH:O	2.06	0.56
1:A:1132:LEU:HD22	2:A:1301:PNS:H302	1.86	0.56
1:C:1118:GLU:O	1:C:1122:ARG:HG3	2.06	0.56
1:D:990:ARG:NH2	3:D:1409:HOH:O	2.38	0.56
1:C:1064:LEU:C	1:C:1064:LEU:HD23	2.31	0.55
1:D:1036:LEU:HD11	1:D:1038:LEU:HD11	1.87	0.55
1:B:1102:VAL:HG11	2:B:1301:PNS:H431	1.88	0.55
1:A:1054:ARG:HH11	1:A:1054:ARG:HG2	1.73	0.54
1:B:772:VAL:HG21	1:B:1132:LEU:HG	1.89	0.54
1:B:779:ARG:HD2	1:B:785:ARG:NE	2.23	0.54
1:C:1064:LEU:HD23	1:C:1064:LEU:O	2.08	0.54
1:B:1147:ARG:NH1	1:B:1152:SER:O	2.41	0.54
1:A:1064:LEU:HD23	1:A:1064:LEU:O	2.09	0.53
1:A:781:ARG:C	1:A:783:SER:H	2.16	0.53
1:A:857:ALA:HB2	1:A:938:VAL:HG11	1.90	0.53
1:C:1072:GLY:HA3	1:C:1111:LEU:HD13	1.91	0.53
1:A:743:LEU:HD12	1:A:802:LEU:HD23	1.87	0.53
1:A:1111:LEU:HA	1:A:1120:ARG:NH2	2.24	0.53
1:C:1102:VAL:HG11	2:C:1301:PNS:S44	2.49	0.52
1:B:767:ASP:HB2	1:B:770:ARG:CD	2.40	0.52
1:B:1102:VAL:HG11	2:B:1301:PNS:S44	2.50	0.52
1:A:799:GLU:O	1:A:803:GLU:HG2	2.09	0.52
1:D:857:ALA:HB2	1:D:938:VAL:HG11	1.91	0.52
1:B:737:ASP:HB3	1:B:738:PRO:HD3	1.91	0.52
1:A:1066:ALA:HB2	1:A:1229:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:VAL:HG21	1:A:1132:LEU:HG	1.92	0.52
1:C:1072:GLY:HA3	1:C:1111:LEU:CD1	2.40	0.51
1:A:783:SER:O	1:A:810:PRO:C	2.54	0.50
1:A:745:GLN:O	1:A:748:GLN:HG2	2.12	0.48
1:B:1036:LEU:HD21	1:B:1219:GLU:HG2	1.95	0.48
1:B:1064:LEU:HD21	1:B:1107:LEU:HD22	1.96	0.47
1:D:1162:ALA:O	2:D:1301:PNS:H372	2.14	0.47
1:A:761:PHE:CE1	1:A:766:GLY:HA3	2.49	0.47
1:C:877:ARG:HH12	1:C:879:GLU:HB2	1.79	0.47
1:A:761:PHE:CE2	1:A:774:LEU:HD22	2.49	0.47
1:B:1072:GLY:HA3	1:B:1111:LEU:CD1	2.45	0.47
1:C:781:ARG:HD2	3:C:1435:HOH:O	2.14	0.47
1:A:761:PHE:HE2	1:A:774:LEU:HD22	1.79	0.47
1:D:1036:LEU:HD13	1:D:1038:LEU:HG	1.97	0.47
1:D:741:GLN:HG2	1:D:745:GLN:HE22	1.80	0.47
1:A:775:LEU:CD1	1:A:786:VAL:HB	2.46	0.46
1:C:1036:LEU:HD13	1:C:1038:LEU:HG	1.98	0.46
1:B:779:ARG:CD	1:B:785:ARG:HG3	2.46	0.46
1:B:762:TYR:HA	1:B:766:GLY:CA	2.46	0.46
1:D:1072:GLY:HA3	1:D:1111:LEU:CD1	2.45	0.46
1:D:1064:LEU:HD23	1:D:1064:LEU:O	2.16	0.45
1:B:1036:LEU:HD13	1:B:1215:LEU:HD11	1.98	0.45
1:A:1173:ALA:CA	3:A:1402:HOH:O	2.64	0.45
1:B:766:GLY:O	1:B:770:ARG:HD3	2.16	0.45
1:C:888:HIS:HB3	3:C:1557:HOH:O	2.14	0.45
1:A:1185:PRO:HD3	1:B:917:ARG:HG2	1.98	0.45
1:B:736:SER:O	1:B:739:LEU:N	2.50	0.45
1:B:803:GLU:HG3	1:B:807:GLN:HE21	1.82	0.45
1:B:1051:LEU:HD11	1:B:1232:ASN:HB3	1.99	0.45
1:C:1033:GLY:HA3	1:C:1186:GLY:HA2	1.99	0.45
1:B:1102:VAL:HG11	2:B:1301:PNS:C43	2.46	0.45
1:C:1045:HIS:CE1	1:C:1049:ARG:HD2	2.52	0.45
1:A:1158:ILE:HD12	1:A:1191:LEU:HB3	1.97	0.44
1:C:803:GLU:HG3	1:C:807:GLN:HE21	1.82	0.44
1:D:772:VAL:HG21	1:D:1132:LEU:HG	1.99	0.44
1:B:802:LEU:HD11	1:B:806:ARG:HE	1.83	0.44
1:D:888:HIS:HB3	3:D:1408:HOH:O	2.18	0.44
1:D:1194:TRP:HH2	2:D:1301:PNS:H44	1.65	0.44
1:A:1072:GLY:HA3	1:A:1111:LEU:CD1	2.47	0.44
1:B:1074:GLU:HG3	1:B:1221:LEU:CD2	2.47	0.44
1:B:1176:ARG:NH2	1:B:1178:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:774:LEU:HD23	1:B:774:LEU:C	2.42	0.44
1:C:1106:PRO:HG3	1:C:1154:LEU:HD21	2.00	0.44
1:D:872:VAL:O	1:D:876:ARG:HG3	2.18	0.44
1:D:743:LEU:C	1:D:743:LEU:HD23	2.43	0.43
1:A:773:HIS:CE1	1:A:1095:GLN:HE22	2.36	0.43
1:B:737:ASP:HB3	1:B:738:PRO:CD	2.47	0.43
1:B:872:VAL:O	1:B:876:ARG:HG3	2.18	0.43
1:C:743:LEU:HD23	1:C:743:LEU:C	2.44	0.43
1:A:1220:ARG:NH1	1:D:866:GLN:HG2	2.33	0.43
1:A:803:GLU:HA	1:A:806:ARG:HG2	2.00	0.43
1:A:1227:ARG:NH2	1:D:862:GLN:OE1	2.52	0.43
1:B:802:LEU:CD1	1:B:806:ARG:HE	2.31	0.42
1:B:1064:LEU:HD21	1:B:1107:LEU:CD2	2.49	0.42
1:C:1036:LEU:CD1	1:C:1038:LEU:CD1	2.98	0.42
1:A:803:GLU:O	1:A:806:ARG:HG2	2.19	0.42
1:D:1194:TRP:HH2	2:D:1301:PNS:S44	2.42	0.42
1:B:802:LEU:HD11	1:B:806:ARG:NE	2.34	0.42
1:D:1008:ALA:HB3	1:D:1149:ARG:NH1	2.34	0.42
1:C:1036:LEU:CD1	1:C:1038:LEU:HD11	2.48	0.42
2:B:1301:PNS:H431	3:B:1545:HOH:O	2.19	0.42
2:B:1301:PNS:H371	2:B:1301:PNS:H32	1.82	0.42
1:A:743:LEU:C	1:A:743:LEU:HD23	2.45	0.42
1:A:872:VAL:O	1:A:876:ARG:HG3	2.20	0.42
1:A:1132:LEU:CD2	2:A:1301:PNS:H302	2.50	0.42
1:B:1074:GLU:HG3	1:B:1221:LEU:HD21	2.01	0.42
1:B:743:LEU:HD23	1:B:743:LEU:C	2.45	0.41
1:D:803:GLU:HG3	1:D:807:GLN:OE1	2.20	0.41
1:A:1091:ARG:NE	1:A:1093:GLU:OE2	2.53	0.41
1:D:741:GLN:HG2	1:D:745:GLN:NE2	2.36	0.41
2:D:1301:PNS:H371	2:D:1301:PNS:C42	2.50	0.41
1:C:737:ASP:HA	1:C:738:PRO:HD3	1.93	0.41
1:C:1014:LEU:HD12	1:C:1014:LEU:N	2.35	0.41
1:C:1139:LEU:HD11	1:C:1154:LEU:HD23	2.01	0.41
1:C:872:VAL:O	1:C:876:ARG:HG3	2.20	0.41
1:C:877:ARG:NH1	1:C:879:GLU:HB2	2.36	0.41
1:C:1162:ALA:HB3	2:C:1301:PNS:C30	2.51	0.41
1:B:958:ASP:HB2	2:B:1301:PNS:C43	2.45	0.40
1:C:1195:LEU:HD22	1:C:1195:LEU:N	2.36	0.40
1:B:1010:ARG:HD3	3:B:1407:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	432/523 (83%)	424 (98%)	6 (1%)	2 (0%)	24	27
1	B	440/523 (84%)	434 (99%)	4 (1%)	2 (0%)	24	27
1	C	448/523 (86%)	442 (99%)	6 (1%)	0	100	100
1	D	435/523 (83%)	431 (99%)	4 (1%)	0	100	100
All	All	1755/2092 (84%)	1731 (99%)	20 (1%)	4 (0%)	43	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	782	LEU
1	A	742	ALA
1	B	737	ASP
1	B	767	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	341/390 (87%)	326 (96%)	15 (4%)	25	34
1	B	343/390 (88%)	332 (97%)	11 (3%)	34	47
1	C	349/390 (90%)	341 (98%)	8 (2%)	44	59
1	D	341/390 (87%)	333 (98%)	8 (2%)	44	59
All	All	1374/1560 (88%)	1332 (97%)	42 (3%)	35	48

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	751	LEU
1	A	775	LEU
1	A	779	ARG
1	A	782	LEU
1	A	799	GLU
1	A	831	LEU
1	A	883	ASP
1	A	954	TYR
1	A	958	ASP
1	A	1041	SER
1	A	1054	ARG
1	A	1056	SER
1	A	1128	LEU
1	A	1194	TRP
1	A	1229	LEU
1	B	736	SER
1	B	770	ARG
1	B	829	ARG
1	B	831	LEU
1	B	947	LEU
1	B	954	TYR
1	B	958	ASP
1	B	1034	GLN
1	B	1097	LEU
1	B	1133	GLU
1	B	1149	ARG
1	C	811	GLU
1	C	831	LEU
1	C	954	TYR
1	C	958	ASP
1	C	1036	LEU
1	C	1128	LEU
1	C	1158	ILE
1	C	1200	GLN
1	D	831	LEU
1	D	897	LEU
1	D	954	TYR
1	D	958	ASP
1	D	1036	LEU
1	D	1071	LEU
1	D	1115	GLN
1	D	1128	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	748	GLN
1	A	986	GLN
1	A	1045	HIS
1	A	1095	GLN
1	A	1123	GLN
1	A	1216	HIS
1	B	750	GLN
1	B	759	GLN
1	B	807	GLN
1	B	893	HIS
1	B	1045	HIS
1	B	1123	GLN
1	B	1134	HIS
1	B	1163	HIS
1	C	759	GLN
1	C	780	GLN
1	C	807	GLN
1	C	1123	GLN
1	C	1200	GLN
1	C	1216	HIS
1	C	1232	ASN
1	D	1134	HIS

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](#)

4 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	PNS	C	1301	1	14,20,21	0.56	0	18,26,29	1.29	2 (11%)
2	PNS	A	1301	1	14,20,21	0.42	0	18,26,29	0.57	0
2	PNS	D	1301	1	14,20,21	0.55	0	18,26,29	0.99	1 (5%)
2	PNS	B	1301	1	14,20,21	0.58	0	18,26,29	1.48	2 (11%)

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	C	1301	1	-	10/24/26/27	-
2	PNS	A	1301	1	-	8/24/26/27	-
2	PNS	D	1301	1	-	10/24/26/27	-
2	PNS	B	1301	1	-	17/24/26/27	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	PNS	C37-C38-C39	3.70	118.56	112.39
2	C	1301	PNS	O33-C32-C29	-3.21	102.75	110.18
2	B	1301	PNS	C37-N36-C34	3.03	127.98	122.55
2	C	1301	PNS	C31-C29-C28	2.53	112.39	108.22
2	D	1301	PNS	C42-N41-C39	2.03	126.60	122.82

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	PNS	O33-C32-C34-O35
2	A	1301	PNS	O33-C32-C34-N36

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Mol	Chain	Res	Type	Atoms
2	A	1301	PNS	N36-C37-C38-C39
2	A	1301	PNS	C38-C39-N41-C42
2	A	1301	PNS	O40-C39-N41-C42
2	A	1301	PNS	N41-C42-C43-S44
2	B	1301	PNS	O27-C28-C29-C30
2	B	1301	PNS	C28-C29-C32-C34
2	B	1301	PNS	C30-C29-C32-C34
2	B	1301	PNS	C31-C29-C32-O33
2	B	1301	PNS	C31-C29-C32-C34
2	B	1301	PNS	C32-C34-N36-C37
2	B	1301	PNS	N36-C37-C38-C39
2	B	1301	PNS	C38-C39-N41-C42
2	C	1301	PNS	C29-C32-C34-O35
2	C	1301	PNS	O33-C32-C34-N36
2	C	1301	PNS	N41-C42-C43-S44
2	D	1301	PNS	C28-C29-C32-C34
2	D	1301	PNS	C30-C29-C32-O33
2	D	1301	PNS	C30-C29-C32-C34
2	D	1301	PNS	C31-C29-C32-C34
2	D	1301	PNS	C38-C39-N41-C42
2	D	1301	PNS	O40-C39-N41-C42
2	B	1301	PNS	O40-C39-N41-C42
2	B	1301	PNS	O35-C34-N36-C37
2	C	1301	PNS	O33-C32-C34-O35
2	D	1301	PNS	C31-C29-C32-O33
2	A	1301	PNS	C29-C32-C34-N36
2	C	1301	PNS	C29-C32-C34-N36
2	B	1301	PNS	O33-C32-C34-O35
2	B	1301	PNS	O27-C28-C29-C31
2	C	1301	PNS	O27-C28-C29-C30
2	C	1301	PNS	O27-C28-C29-C31
2	C	1301	PNS	C43-C42-N41-C39
2	B	1301	PNS	N41-C42-C43-S44
2	B	1301	PNS	C28-C29-C32-O33
2	D	1301	PNS	C28-C29-C32-O33
2	C	1301	PNS	O40-C39-N41-C42
2	A	1301	PNS	C29-C32-C34-O35
2	B	1301	PNS	C29-C32-C34-O35
2	B	1301	PNS	C29-C32-C34-N36
2	B	1301	PNS	O33-C32-C34-N36
2	D	1301	PNS	C37-C38-C39-O40
2	D	1301	PNS	C37-C38-C39-N41

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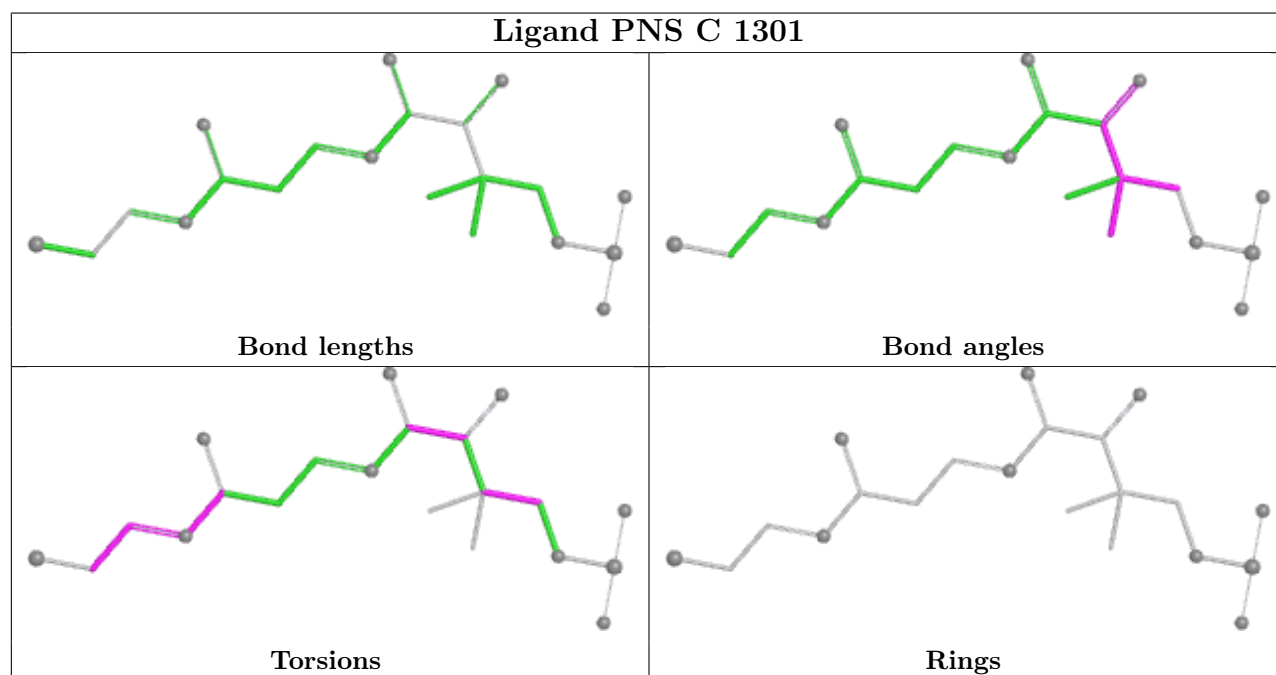
Mol	Chain	Res	Type	Atoms
2	C	1301	PNS	O27-C28-C29-C32

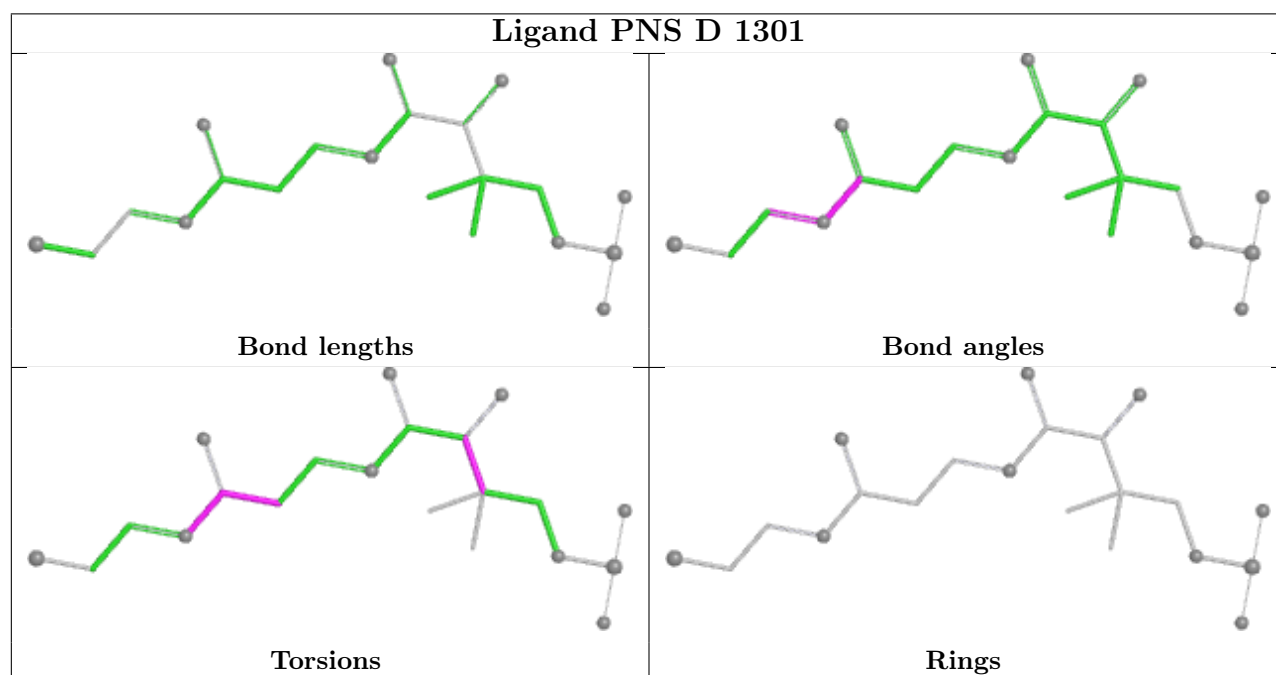
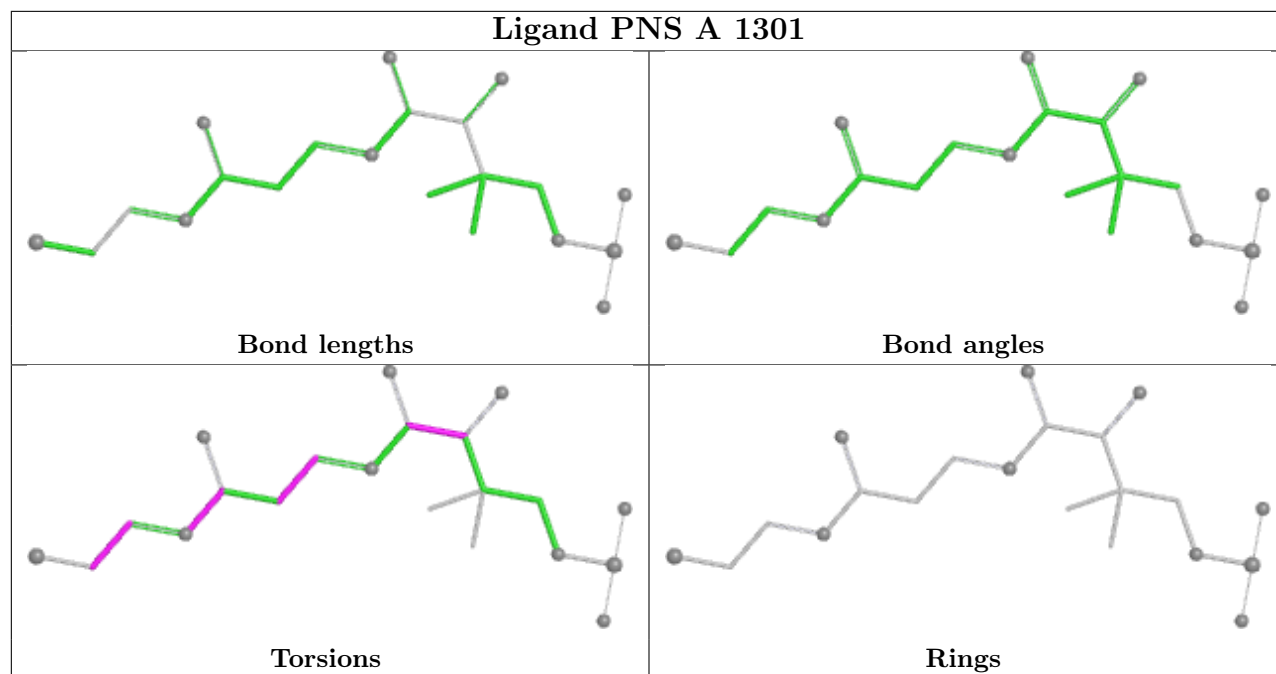
There are no ring outliers.

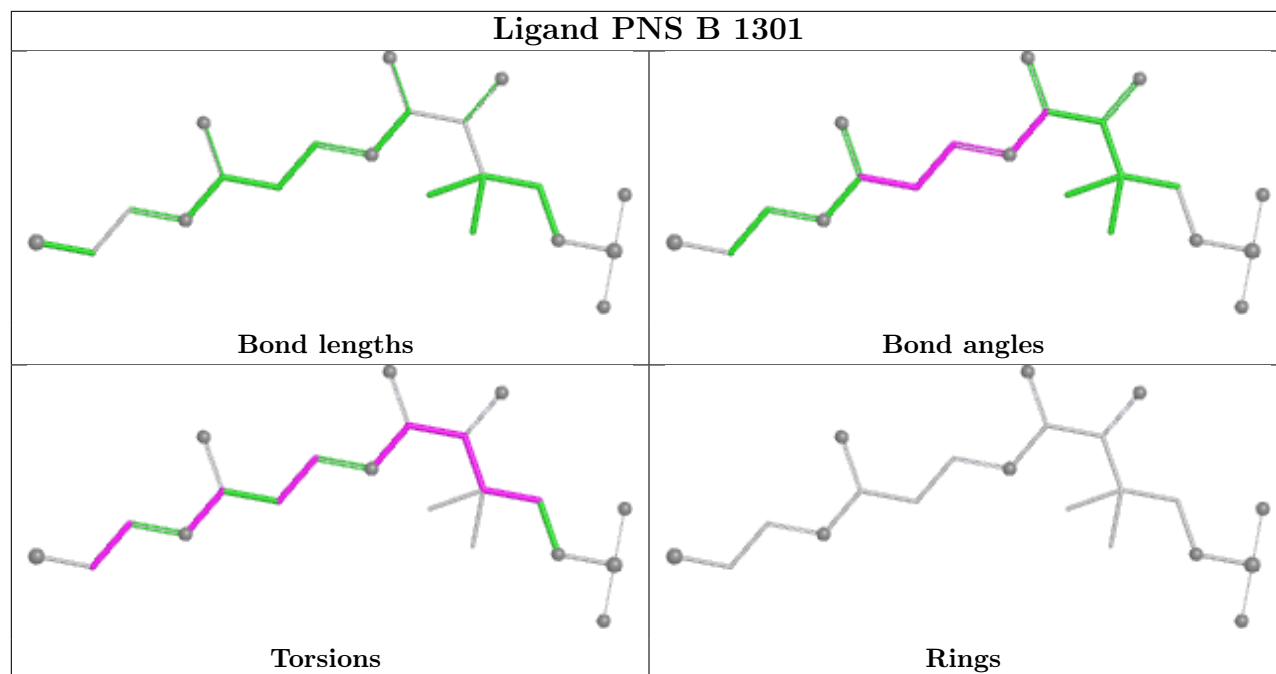
4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1301	PNS	2	0
2	A	1301	PNS	3	0
2	D	1301	PNS	5	0
2	B	1301	PNS	11	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 [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	446/523 (85%)	0.63	71 (15%) 5 3	17, 35, 105, 142	0
1	B	452/523 (86%)	0.28	25 (5%) 30 27	17, 34, 64, 92	0
1	C	458/523 (87%)	0.15	15 (3%) 49 46	19, 33, 58, 91	0
1	D	447/523 (85%)	0.54	31 (6%) 23 20	20, 42, 75, 108	0
All	All	1803/2092 (86%)	0.40	142 (7%) 18 16	17, 36, 75, 142	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	743	LEU	6.5
1	A	753	ALA	5.9
1	A	755	PRO	5.5
1	A	742	ALA	5.5
1	A	754	PRO	5.5
1	A	763	ALA	5.3
1	A	751	LEU	5.3
1	A	747	TRP	5.0
1	B	767	ASP	5.0
1	A	793	GLY	4.9
1	A	764	ALA	4.9
1	D	1119	TRP	4.8
1	A	809	ALA	4.8
1	A	1113	PRO	4.8
1	A	804	LEU	4.7
1	A	786	VAL	4.4
1	A	749	ALA	4.4
1	A	805	LEU	4.4
1	A	801	LEU	4.4
1	A	744	HIS	4.3
1	A	802	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	1117	VAL	4.1
1	A	798	PRO	4.1
1	A	800	ALA	4.0
1	C	1113	PRO	4.0
1	A	810	PRO	3.8
1	A	780	GLN	3.8
1	A	765	GLY	3.8
1	C	1186	GLY	3.8
1	B	1163	HIS	3.7
1	A	797	THR	3.7
1	B	821	ALA	3.6
1	D	808	ALA	3.6
1	A	746	ALA	3.6
1	D	1113	PRO	3.6
1	B	766	GLY	3.6
1	A	781	ARG	3.6
1	D	1077	VAL	3.6
1	C	1114	GLU	3.5
1	A	1173	ALA	3.5
1	A	760	GLY	3.5
1	B	765	GLY	3.5
1	A	783	SER	3.4
1	B	752	GLY	3.4
1	B	1234	GLY	3.4
1	D	809	ALA	3.4
1	B	794	GLY	3.4
1	A	787	PRO	3.3
1	B	736	SER	3.3
1	A	1201	GLY	3.3
1	A	775	LEU	3.3
1	A	761	PHE	3.3
1	D	810	PRO	3.1
1	A	784	ARG	3.1
1	A	785	ARG	3.1
1	C	1164	ASN	3.1
1	A	1198	GLN	3.1
1	A	782	LEU	3.1
1	B	753	ALA	3.0
1	A	741	GLN	3.0
1	D	880	THR	3.0
1	A	1119	TRP	3.0
1	A	776	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	762	TYR	2.9
1	A	808	ALA	2.9
1	C	880	THR	2.9
1	A	752	GLY	2.9
1	C	1033	GLY	2.9
1	B	797	THR	2.9
1	C	1112	ARG	2.8
1	D	1154	LEU	2.8
1	D	1075	LEU	2.8
1	A	1150	GLY	2.8
1	D	785	ARG	2.7
1	B	1112	ARG	2.7
1	C	822	ALA	2.7
1	C	1234	GLY	2.7
1	C	1199	PRO	2.7
1	A	1115	GLN	2.6
1	A	799	GLU	2.6
1	B	1197	ASP	2.6
1	A	766	GLY	2.6
1	D	941	ASP	2.6
1	A	778	LEU	2.6
1	A	1197	ASP	2.6
1	A	774	LEU	2.6
1	B	795	PRO	2.6
1	A	1053	GLU	2.5
1	A	1163	HIS	2.5
1	A	1233	ALA	2.5
1	A	1186	GLY	2.5
1	C	1115	GLN	2.5
1	D	1114	GLU	2.5
1	D	1033	GLY	2.5
1	A	1112	ARG	2.5
1	A	1114	GLU	2.5
1	B	1054	ARG	2.5
1	C	894	ALA	2.5
1	A	777	THR	2.4
1	A	1188	ARG	2.4
1	D	1120	ARG	2.4
1	D	1194	TRP	2.4
1	A	740	GLU	2.4
1	D	1076	GLY	2.4
1	D	1116	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1010	ARG	2.4
1	A	1009	GLU	2.4
1	A	1051	LEU	2.3
1	B	1114	GLU	2.3
1	D	1014	LEU	2.3
1	D	1233	ALA	2.3
1	D	1055	THR	2.3
1	D	1112	ARG	2.3
1	C	990	ARG	2.3
1	A	790	ALA	2.2
1	A	792	ALA	2.2
1	B	808	ALA	2.2
1	B	1032	ALA	2.2
1	D	1152	SER	2.2
1	D	1146	LEU	2.2
1	D	1079	ASP	2.2
1	A	748	GLN	2.2
1	A	1015	ALA	2.2
1	B	757	ALA	2.2
1	B	880	THR	2.2
1	B	756	ARG	2.1
1	D	1054	ARG	2.1
1	A	1155	PRO	2.1
1	B	803	GLU	2.1
1	B	744	HIS	2.1
1	A	1202	TRP	2.1
1	C	1152	SER	2.1
1	C	1015	ALA	2.1
1	D	1150	GLY	2.1
1	D	807	GLN	2.0
1	B	751	LEU	2.0
1	A	1117	VAL	2.0
1	A	1149	ARG	2.0
1	D	1149	ARG	2.0
1	B	1015	ALA	2.0
1	D	787	PRO	2.0
1	D	999	ARG	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 [i](#)

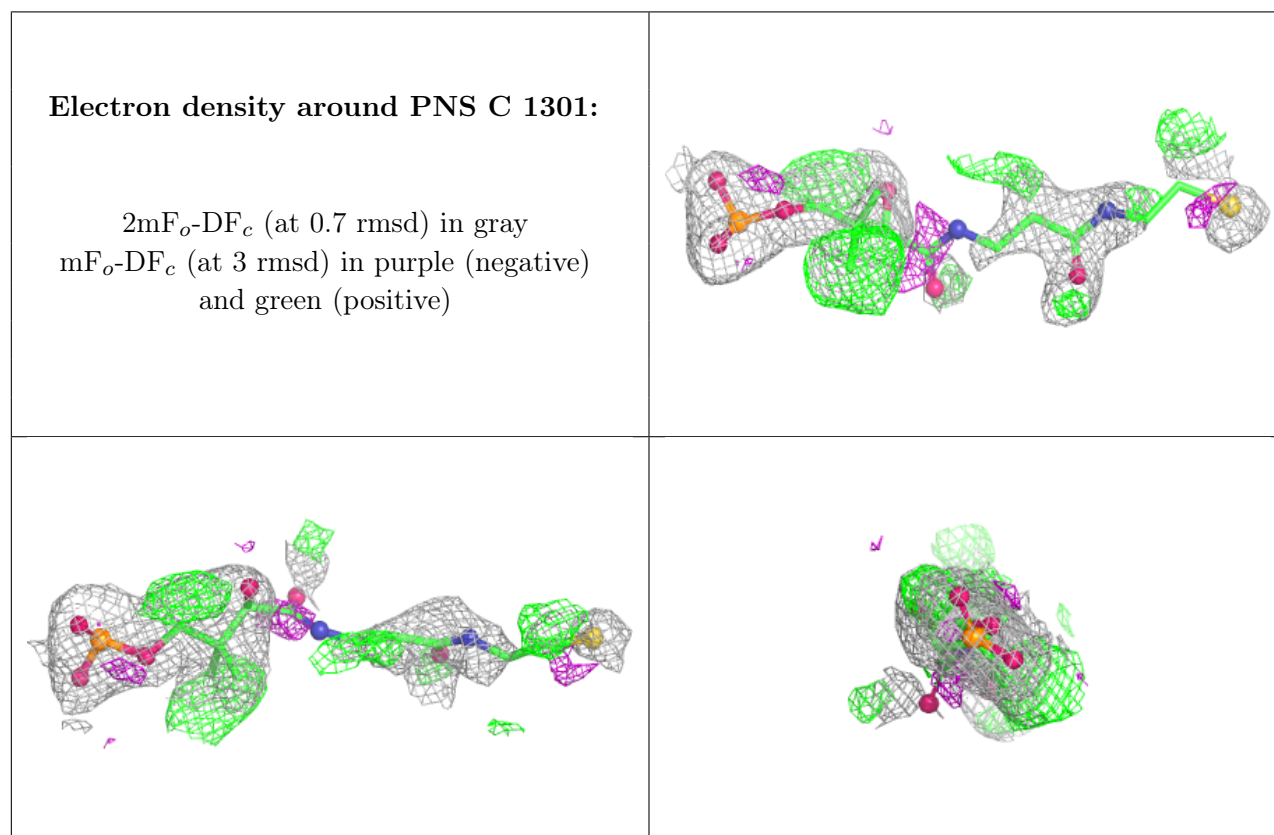
There are no oligosaccharides in this entry.

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.

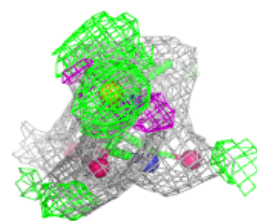
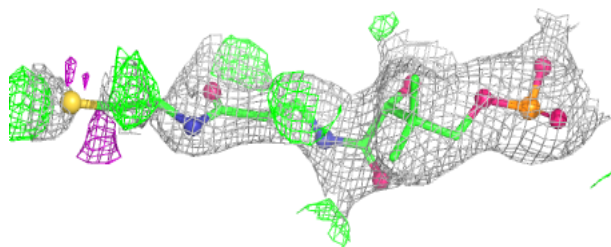
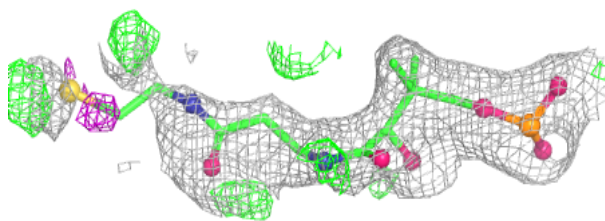
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PNS	C	1301	21/22	0.82	0.25	29,69,89,97	0
2	PNS	B	1301	21/22	0.87	0.19	32,60,89,102	0
2	PNS	A	1301	21/22	0.87	0.18	48,59,93,93	0
2	PNS	D	1301	21/22	0.90	0.13	35,46,62,84	0

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.

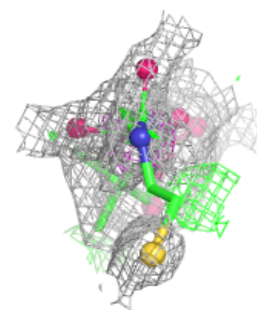
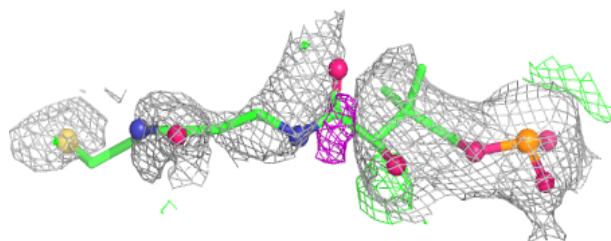
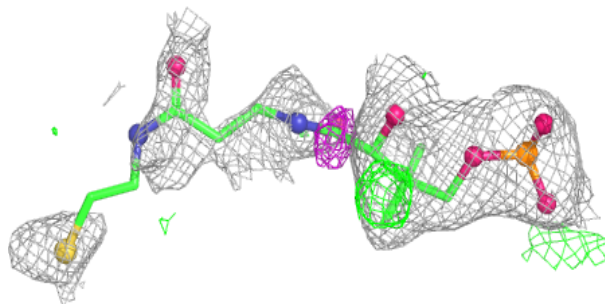


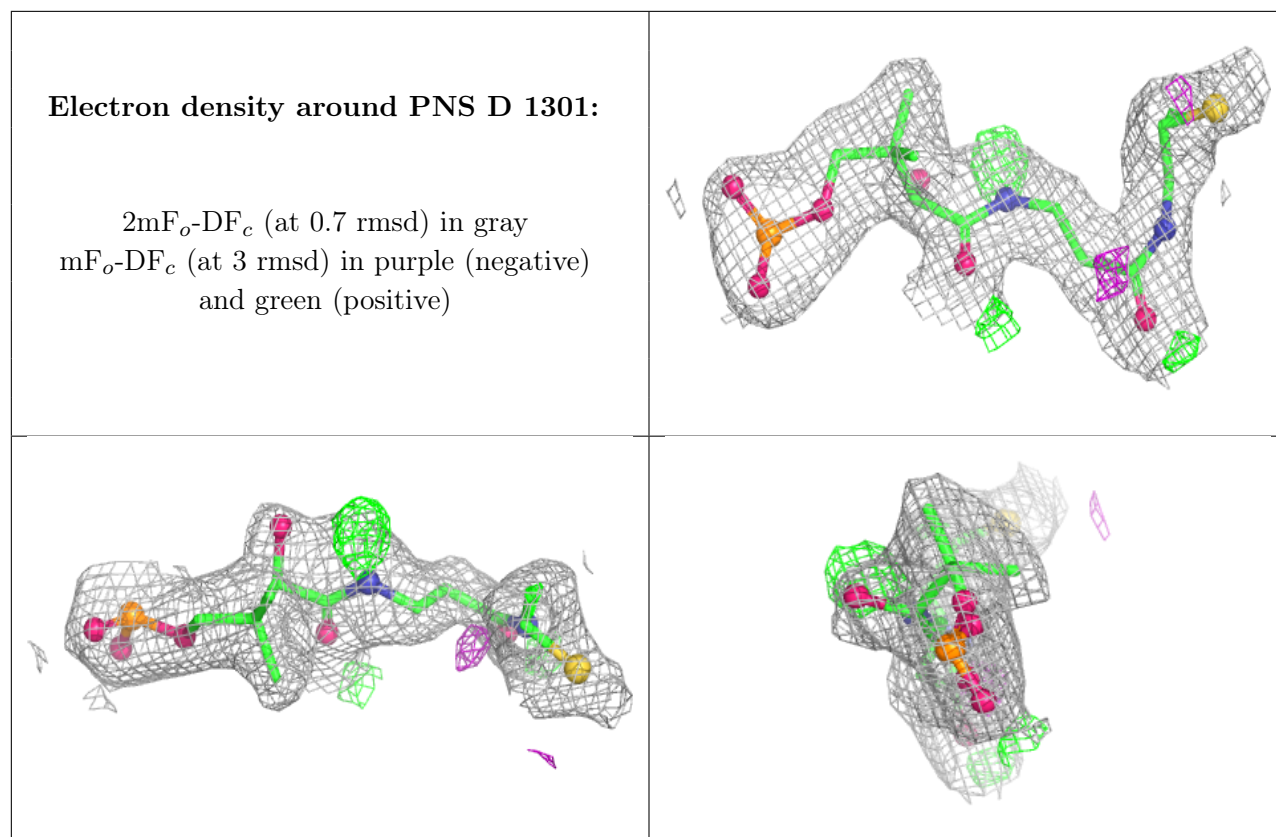
Electron density around PNS B 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PNS A 1301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.