



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2022 – 12:07 AM JST

PDB ID : 7X0F
Title : Structure of Pseudomonas NRPS protein, AmbB-TC bound to Ppant
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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 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 : 2.28.1
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) : 2.28.1

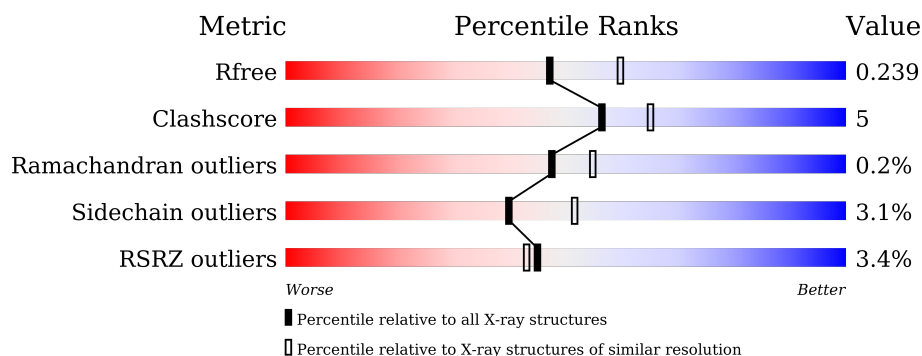
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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	<div> <div>9%</div> <div>74%</div> <div>10%</div> <div>15%</div> </div>
1	B	523	<div> <div>%</div> <div>77%</div> <div>8%</div> <div>14%</div> </div>
1	C	523	<div> <div>%</div> <div>80%</div> <div>7%</div> <div>12%</div> </div>
1	D	523	<div> <div>%</div> <div>79%</div> <div>7%</div> <div>15%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PNS	B	1301	-	-	X	-

2 Entry composition [i](#)

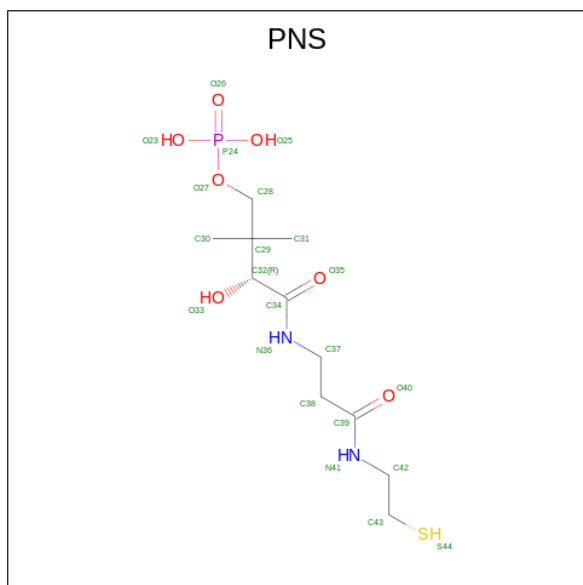
There are 3 unique types of molecules in this entry. The entry contains 14566 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$) (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		

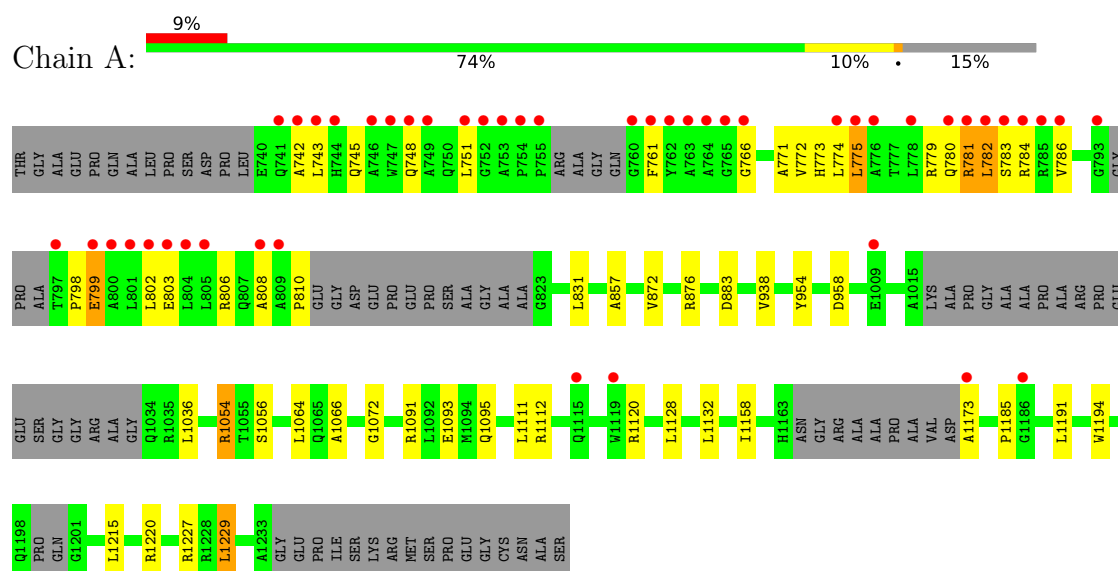
- Molecule 3 is water.

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		

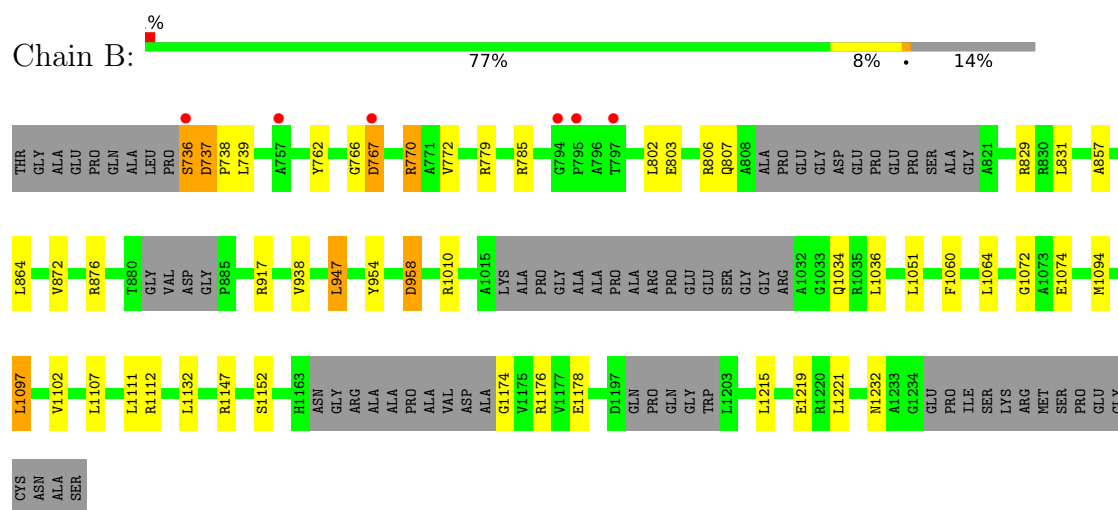
3 Residue-property plots

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.

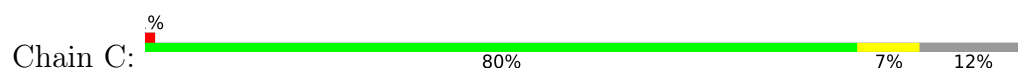
• Molecule 1: AMB antimetabolite synthase AmbB

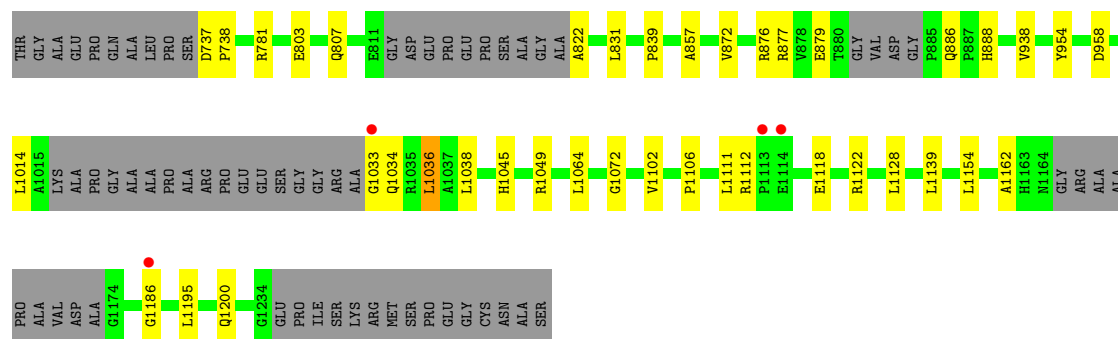


• Molecule 1: AMB antimetabolite synthase AmbB

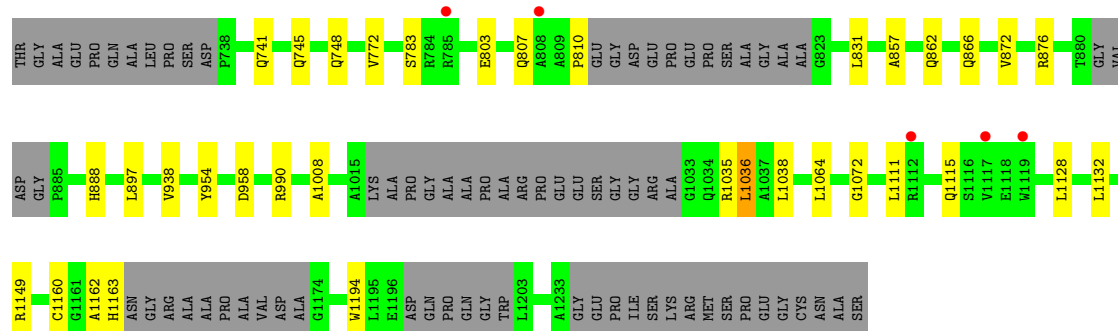
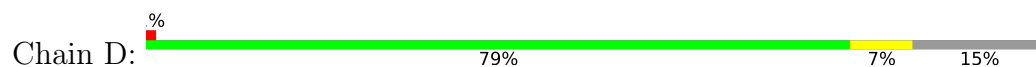


• Molecule 1: AMB antimetabolite synthase AmbB





- 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 75.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.56-2.20) 98.8 (75.25-2.20)	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 , 0.239	Depositor DCC
R_{free} test set	5662 reflections (4.96%)	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)	0.37 , 43.9	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	0.53	0/3482	0.72	0/4731
1	B	0.53	0/3512	0.73	0/4771
1	C	0.52	0/3573	0.70	0/4858
1	D	0.49	0/3484	0.70	0/4733
All	All	0.52	0/14051	0.71	0/19093

There are no bond length outliers.

There are no bond angle outliers.

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	46	0
1	B	3454	0	3519	43	0
1	C	3510	0	3565	28	0
1	D	3425	0	3501	22	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	141	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 (141) 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: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:B:736:SER:O	1:B:737:ASP:C	2.36	0.65
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:ARG:CZ	1:A:781:ARG:HA	2.33	0.58
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: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: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:O	1:A:1064:LEU:HD23	2.09	0.53
1:A:857:ALA:HB2	1:A:938:VAL:HG11	1.90	0.53
1:A:1064:LEU:HD23	1:A:1064:LEU:C	2.29	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
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:D:1064:LEU:C	1:D:1064:LEU:HD23	2.30	0.51
1:C:1064:LEU:HD23	1:C:1064:LEU:C	2.31	0.51
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:D:1194:TRP:HH2	2:D:1301:PNS:H44	1.60	0.48
1:B:1064:LEU:HD21	1:B:1107:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:783:SER:O	1:A:810:PRO:C	2.54	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:A:781:ARG:C	1:A:783:SER:H	2.16	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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%)	29	31
1	B	440/523 (84%)	434 (99%)	4 (1%)	2 (0%)	29	31
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%)	47	55

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%)	324 (95%)	17 (5%)	24	30
1	B	343/390 (88%)	333 (97%)	10 (3%)	42	54
1	C	349/390 (90%)	342 (98%)	7 (2%)	55	69
1	D	341/390 (87%)	332 (97%)	9 (3%)	46	58
All	All	1374/1560 (88%)	1331 (97%)	43 (3%)	40	51

All (43) 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	780	GLN
1	A	781	ARG
1	A	782	LEU
1	A	799	GLU

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Mol	Chain	Res	Type
1	A	831	LEU
1	A	883	ASP
1	A	954	TYR
1	A	958	ASP
1	A	1054	ARG
1	A	1056	SER
1	A	1112	ARG
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	1112	ARG
1	C	831	LEU
1	C	954	TYR
1	C	958	ASP
1	C	1036	LEU
1	C	1112	ARG
1	C	1128	LEU
1	C	1200	GLN
1	D	748	GLN
1	D	831	LEU
1	D	897	LEU
1	D	954	TYR
1	D	958	ASP
1	D	1036	LEU
1	D	1115	GLN
1	D	1128	LEU
1	D	1160	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	748	GLN
1	A	1045	HIS

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Mol	Chain	Res	Type
1	A	1095	GLN
1	A	1123	GLN
1	B	773	HIS
1	B	807	GLN
1	B	1123	GLN
1	B	1144	GLN
1	B	1148	GLN
1	B	1163	HIS
1	C	807	GLN
1	C	866	GLN
1	C	1045	HIS
1	C	1144	GLN
1	C	1200	GLN
1	D	773	HIS
1	D	1163	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 monosaccharides 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	A	1301	1	13,20,21	0.35	0	18,26,29	0.57	0
2	PNS	D	1301	1	13,20,21	0.57	0	18,26,29	1.00	1 (5%)
2	PNS	C	1301	1	13,20,21	0.43	0	18,26,29	1.27	2 (11%)
2	PNS	B	1301	1	13,20,21	0.55	0	18,26,29	1.47	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	A	1301	1	-	8/24/26/27	-
2	PNS	D	1301	1	-	11/24/26/27	-
2	PNS	C	1301	1	-	10/24/26/27	-
2	PNS	B	1301	1	-	16/24/26/27	-

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	3.72	118.56	112.36
2	C	1301	PNS	O33-C32-C29	-3.19	102.75	110.25
2	B	1301	PNS	C37-N36-C34	3.03	127.98	122.59
2	C	1301	PNS	C31-C29-C28	2.55	112.39	108.23
2	D	1301	PNS	C42-N41-C39	2.02	126.60	122.84

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
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	C28-C29-C32-C34
2	B	1301	PNS	C30-C29-C32-C34
2	B	1301	PNS	C31-C29-C32-O33

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

There are no ring outliers.

4 monomers are involved in 21 short contacts:

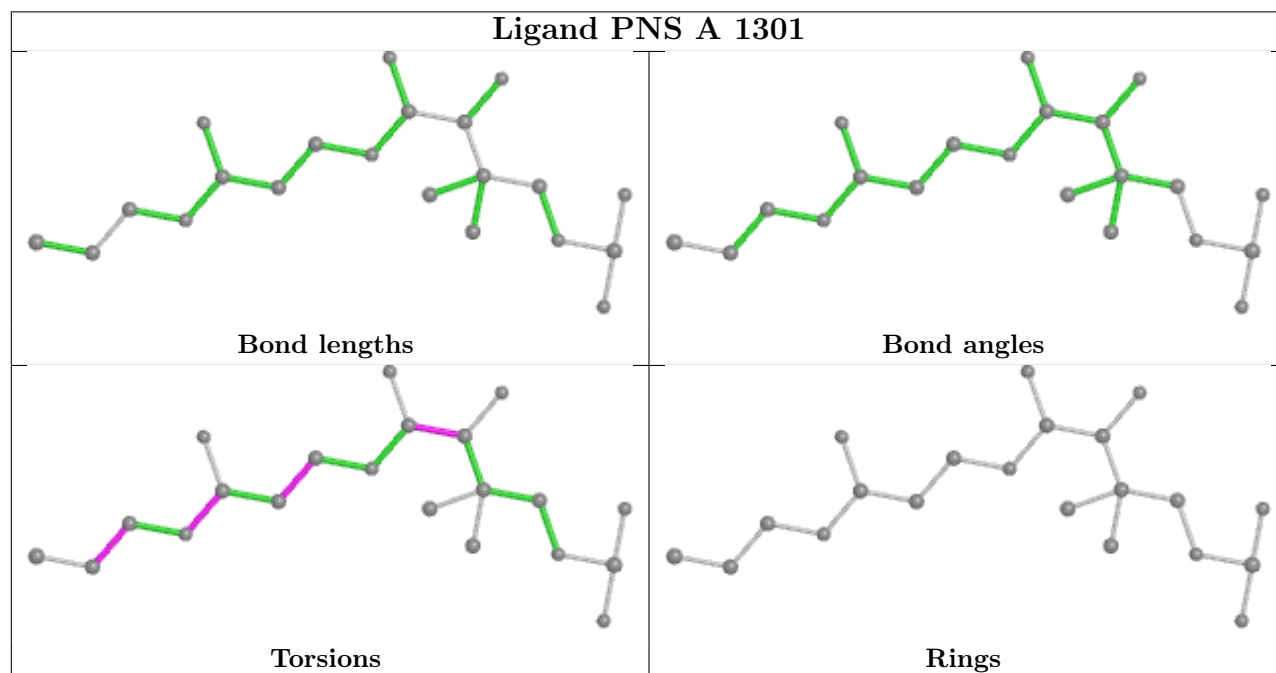
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	PNS	3	0

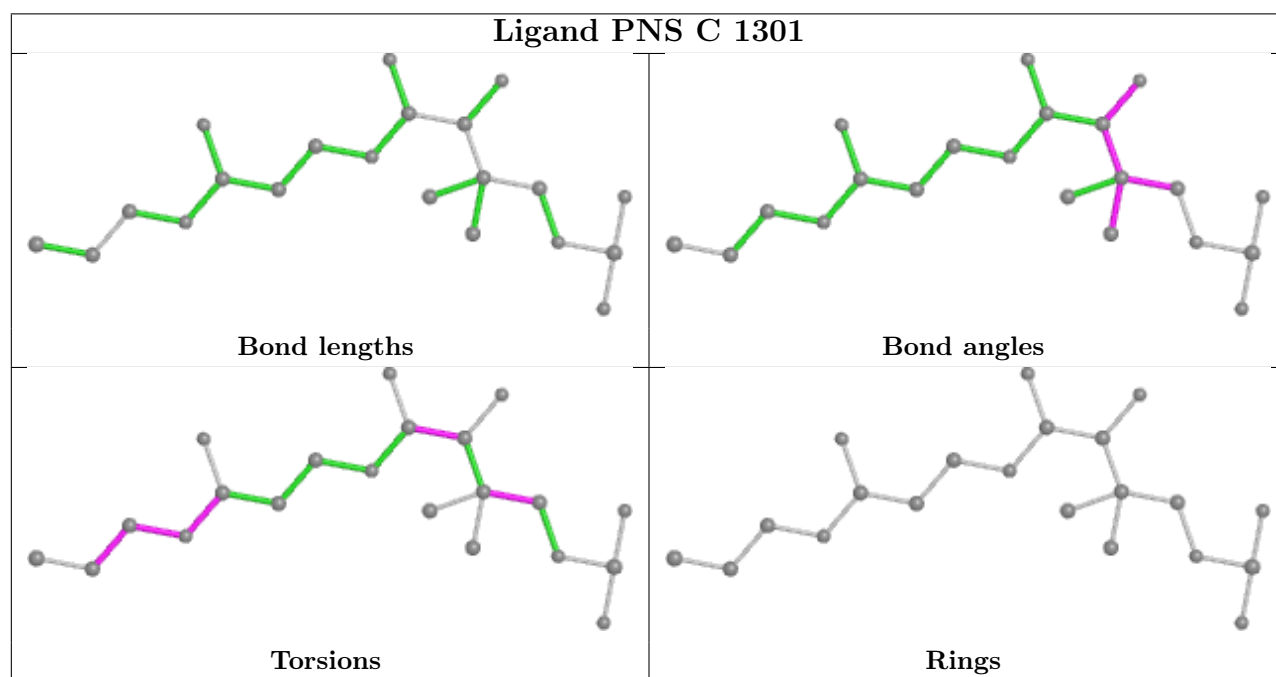
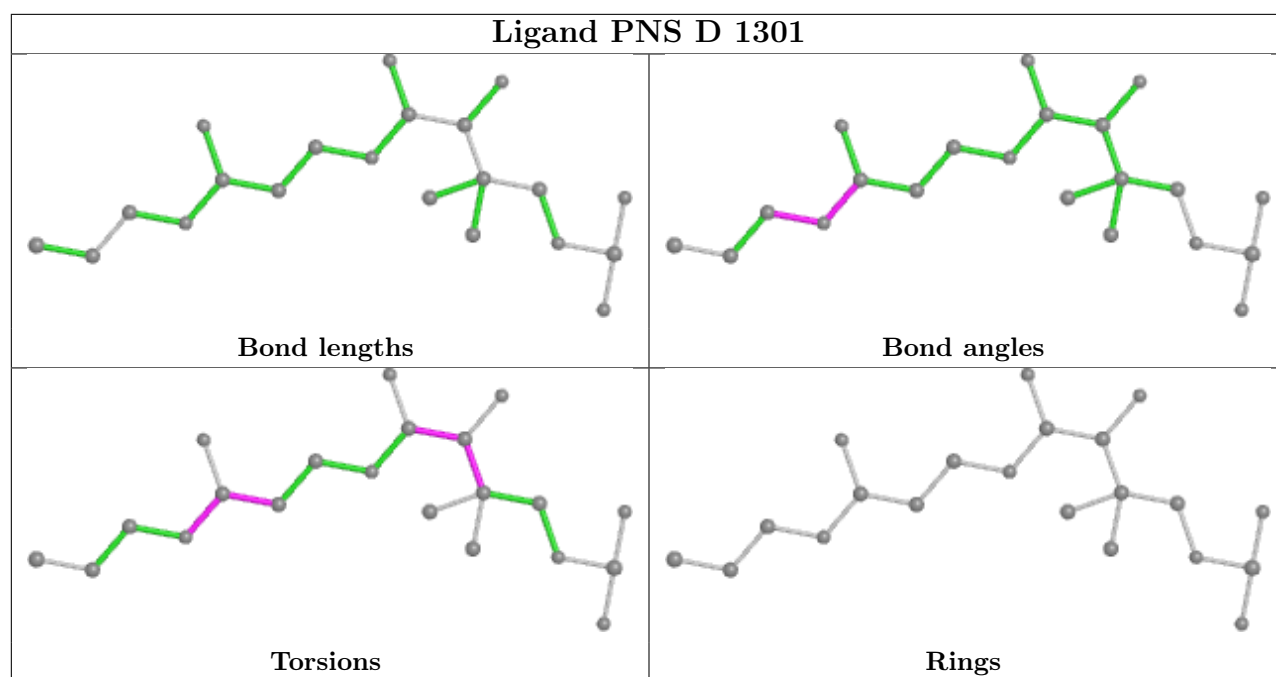
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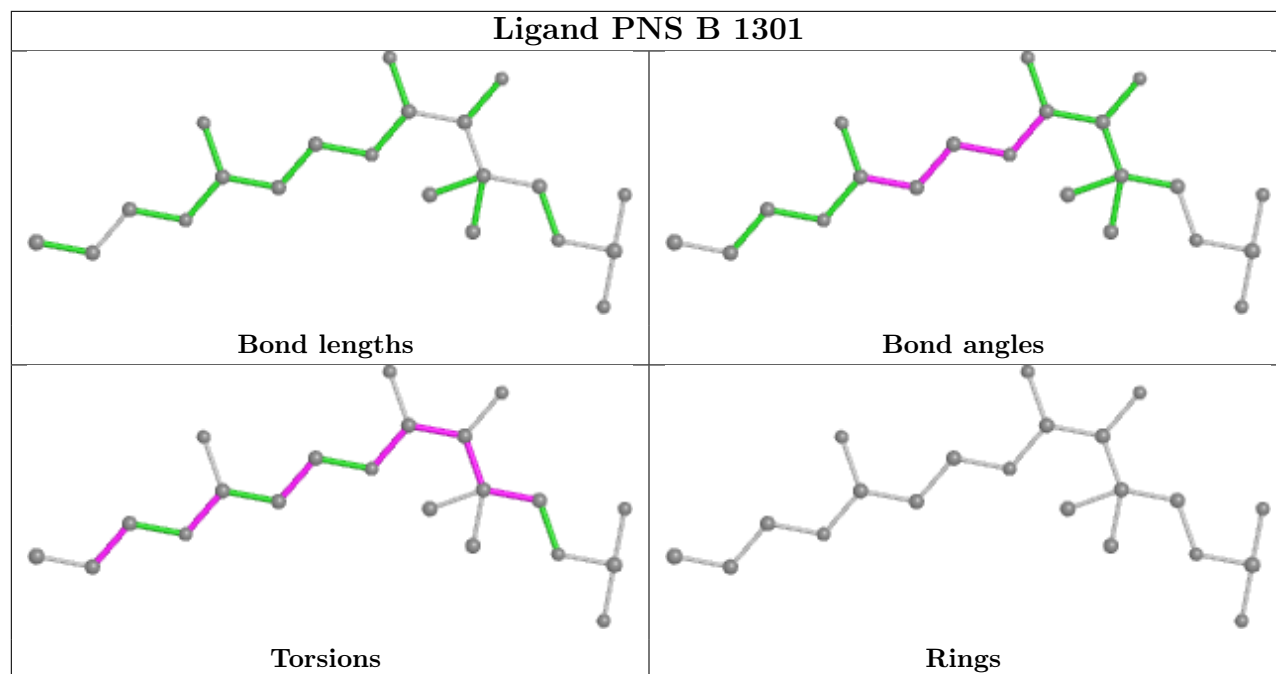
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1301	PNS	5	0
2	C	1301	PNS	2	0
2	B	1301	PNS	11	0

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%)	0.44	47 (10%) 6 5	17, 35, 105, 142	0
1	B	452/523 (86%)	0.08	6 (1%) 77 75	17, 34, 64, 92	0
1	C	458/523 (87%)	-0.01	4 (0%) 84 83	19, 33, 58, 91	0
1	D	447/523 (85%)	0.10	5 (1%) 80 79	20, 42, 75, 108	0
All	All	1803/2092 (86%)	0.15	62 (3%) 45 43	17, 36, 75, 142	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	751	LEU	7.6
1	A	743	LEU	6.2
1	A	809	ALA	6.0
1	A	763	ALA	5.6
1	A	752	GLY	5.6
1	A	765	GLY	5.6
1	A	780	GLN	5.3
1	A	764	ALA	4.7
1	A	800	ALA	4.6
1	A	749	ALA	4.4
1	A	781	ARG	4.3
1	A	744	HIS	4.1
1	A	747	TRP	4.1
1	A	754	PRO	4.1
1	A	802	LEU	4.0
1	A	746	ALA	4.0
1	A	784	ARG	3.9
1	A	783	SER	3.7
1	A	797	THR	3.6
1	B	736	SER	3.6
1	A	762	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	753	ALA	3.5
1	A	761	PHE	3.5
1	A	801	LEU	3.5
1	A	785	ARG	3.4
1	A	755	PRO	3.4
1	A	742	ALA	3.4
1	B	767	ASP	3.1
1	A	766	GLY	3.1
1	C	1113	PRO	3.1
1	A	799	GLU	3.0
1	A	804	LEU	2.8
1	D	1119	TRP	2.8
1	A	1119	TRP	2.8
1	C	1114	GLU	2.7
1	A	741	GLN	2.7
1	A	775	LEU	2.7
1	B	757	ALA	2.7
1	A	776	ALA	2.6
1	A	760	GLY	2.6
1	B	795	PRO	2.6
1	A	793	GLY	2.5
1	A	774	LEU	2.5
1	A	748	GLN	2.5
1	A	803	GLU	2.4
1	A	1186	GLY	2.4
1	A	786	VAL	2.4
1	D	785	ARG	2.3
1	C	1186	GLY	2.3
1	D	1112	ARG	2.3
1	B	794	GLY	2.2
1	A	808	ALA	2.2
1	D	808	ALA	2.2
1	C	1033	GLY	2.2
1	A	1009	GLU	2.2
1	A	778	LEU	2.2
1	A	782	LEU	2.2
1	B	797	THR	2.1
1	A	805	LEU	2.1
1	D	1117	VAL	2.1
1	A	1115	GLN	2.1
1	A	1173	ALA	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](#)

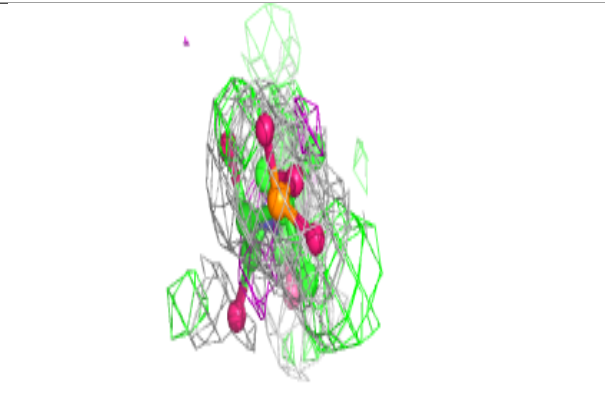
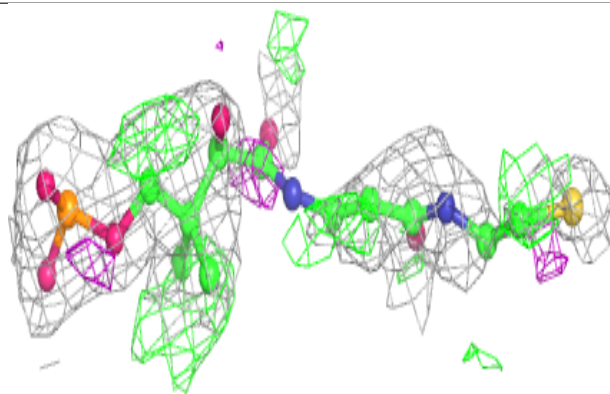
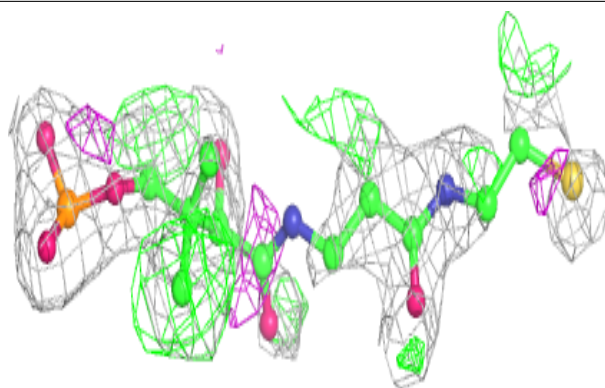
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PNS	C	1301	21/22	0.88	0.24	29,69,89,97	0
2	PNS	A	1301	21/22	0.90	0.24	48,59,93,93	0
2	PNS	B	1301	21/22	0.91	0.20	32,60,89,102	0
2	PNS	D	1301	21/22	0.92	0.16	35,46,62,84	0

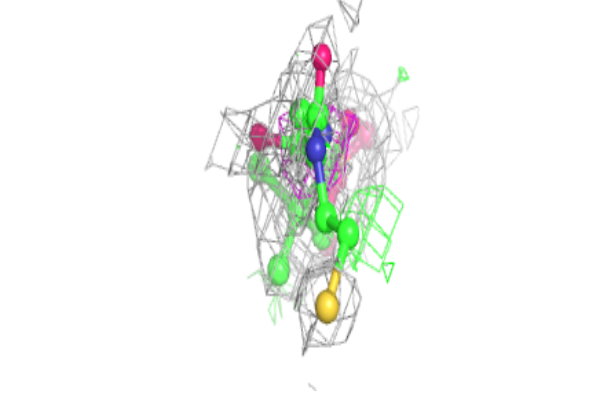
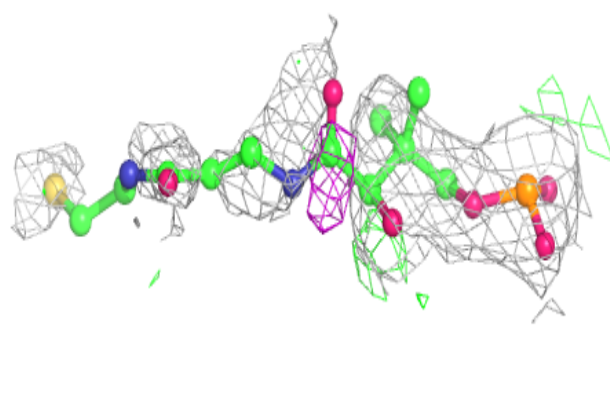
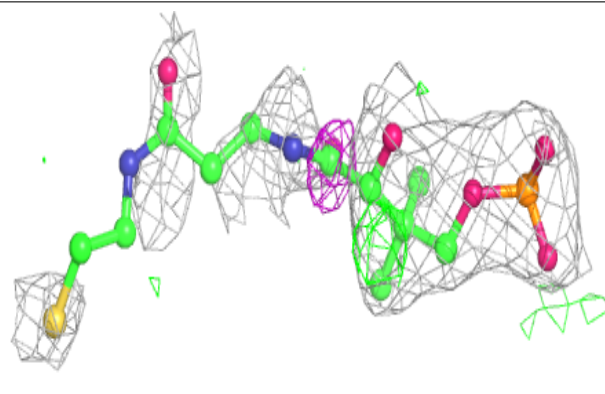
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PNS C 1301:

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

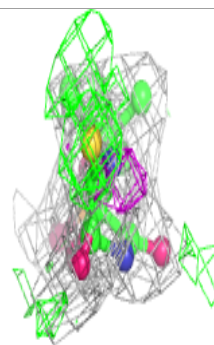
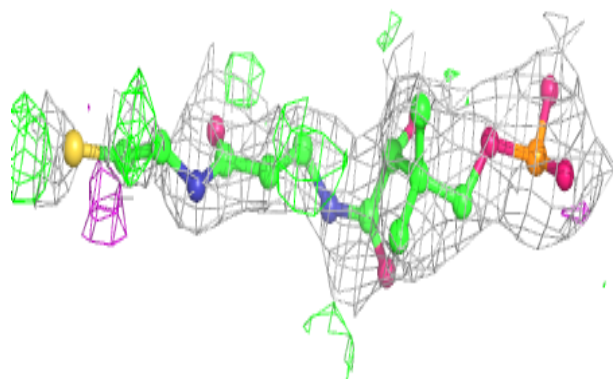
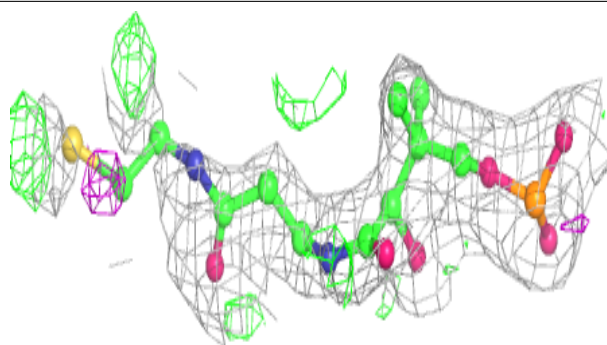
**Electron density around PNS A 1301:**

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

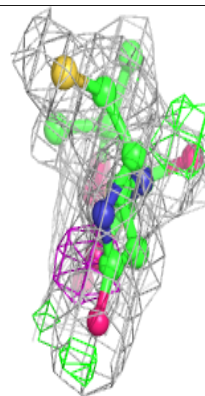
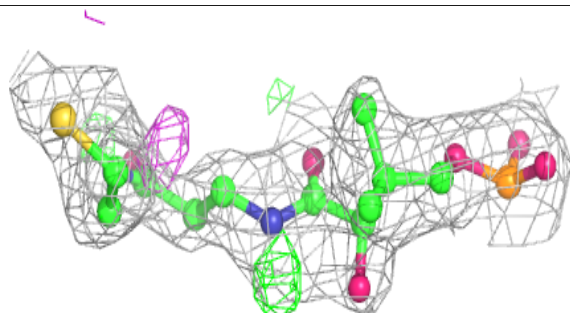
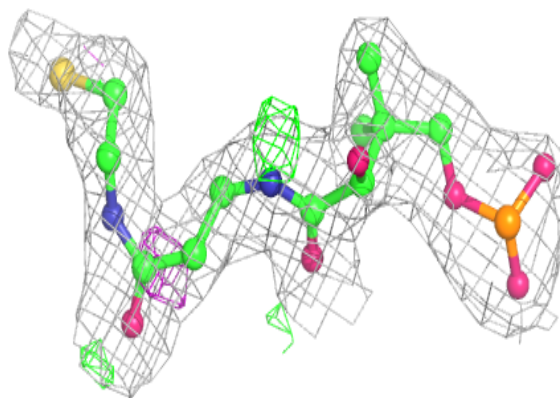


Electron density around PNS B 1301:

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

**Electron density around PNS D 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 [i](#)

There are no such residues in this entry.