



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 06:16 AM EDT

PDB ID : 5OE6  
Title : Crystal structure of the N-terminal domain of PqsA in complex with 6-fluoro anthraniloyl-AMP (crystal form 1)  
Authors : Witzgall, F.; Ewert, W.; Blankenfeldt, W.  
Deposited on : 2017-07-07  
Resolution : 1.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

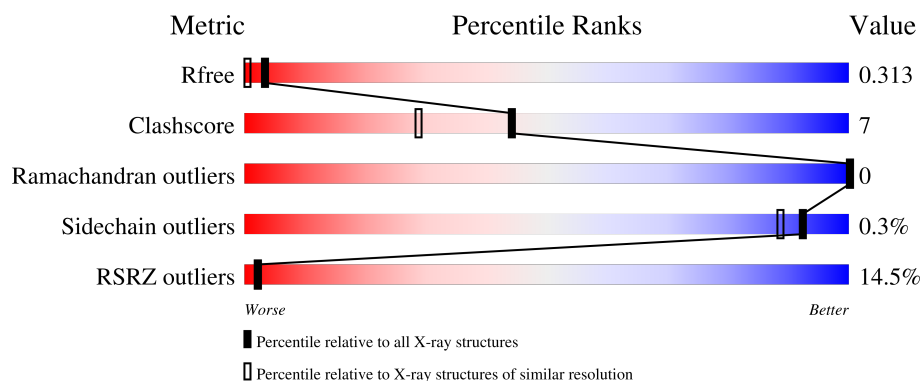
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	407	<div> <div>23%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>
1	B	407	<div> <div>2%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	C	407	<div> <div>28%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
1	D	407	<div> <div>3%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25754 atoms, of which 12038 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 Anthranilate–CoA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	394	Total	C	H	N	O	S	0	8	0
			6073	1947	3017	539	557	13			
1	B	392	Total	C	H	N	O	S	0	6	0
			6054	1937	3012	543	549	13			
1	C	393	Total	C	H	N	O	S	0	5	0
			5985	1923	2964	535	550	13			
1	D	391	Total	C	H	N	O	S	0	3	0
			5970	1919	2959	532	548	12			

There are 32 discrepancies between the modelled and reference sequences:

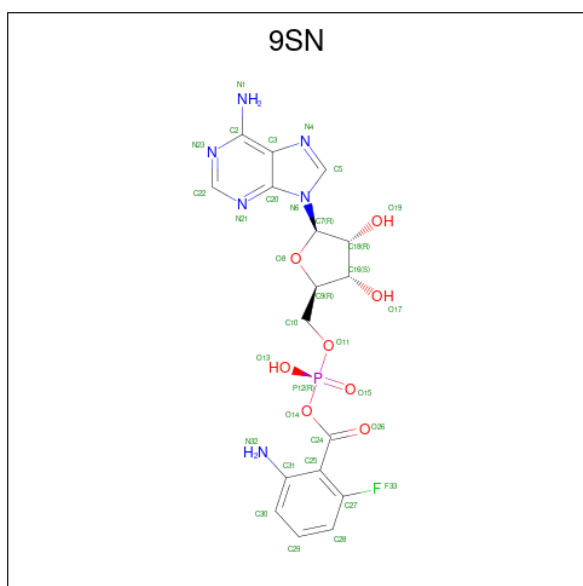
Chain	Residue	Modelled	Actual	Comment	Reference
A	400	LEU	-	expression tag	UNP Q9I4X3
A	401	GLU	-	expression tag	UNP Q9I4X3
A	402	HIS	-	expression tag	UNP Q9I4X3
A	403	HIS	-	expression tag	UNP Q9I4X3
A	404	HIS	-	expression tag	UNP Q9I4X3
A	405	HIS	-	expression tag	UNP Q9I4X3
A	406	HIS	-	expression tag	UNP Q9I4X3
A	407	HIS	-	expression tag	UNP Q9I4X3
B	400	LEU	-	expression tag	UNP Q9I4X3
B	401	GLU	-	expression tag	UNP Q9I4X3
B	402	HIS	-	expression tag	UNP Q9I4X3
B	403	HIS	-	expression tag	UNP Q9I4X3
B	404	HIS	-	expression tag	UNP Q9I4X3
B	405	HIS	-	expression tag	UNP Q9I4X3
B	406	HIS	-	expression tag	UNP Q9I4X3
B	407	HIS	-	expression tag	UNP Q9I4X3
C	400	LEU	-	expression tag	UNP Q9I4X3
C	401	GLU	-	expression tag	UNP Q9I4X3
C	402	HIS	-	expression tag	UNP Q9I4X3
C	403	HIS	-	expression tag	UNP Q9I4X3
C	404	HIS	-	expression tag	UNP Q9I4X3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	405	HIS	-	expression tag	UNP Q9I4X3
C	406	HIS	-	expression tag	UNP Q9I4X3
C	407	HIS	-	expression tag	UNP Q9I4X3
D	400	LEU	-	expression tag	UNP Q9I4X3
D	401	GLU	-	expression tag	UNP Q9I4X3
D	402	HIS	-	expression tag	UNP Q9I4X3
D	403	HIS	-	expression tag	UNP Q9I4X3
D	404	HIS	-	expression tag	UNP Q9I4X3
D	405	HIS	-	expression tag	UNP Q9I4X3
D	406	HIS	-	expression tag	UNP Q9I4X3
D	407	HIS	-	expression tag	UNP Q9I4X3

- Molecule 2 is 6-fluoroanthraniloyl-AMP (three-letter code: 9SN) (formula:  $C_{17}H_{18}FN_6O_8P$ ).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	P	0	0
			51	17	1	18	6	8	1		
2	B	1	Total	C	F	H	N	O	P	0	0
			51	17	1	18	6	8	1		
2	C	1	Total	C	F	H	N	O	P	0	0
			51	17	1	18	6	8	1		
2	D	1	Total	C	F	H	N	O	P	0	0
			51	17	1	18	6	8	1		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	0	0
			24	6	14	4		

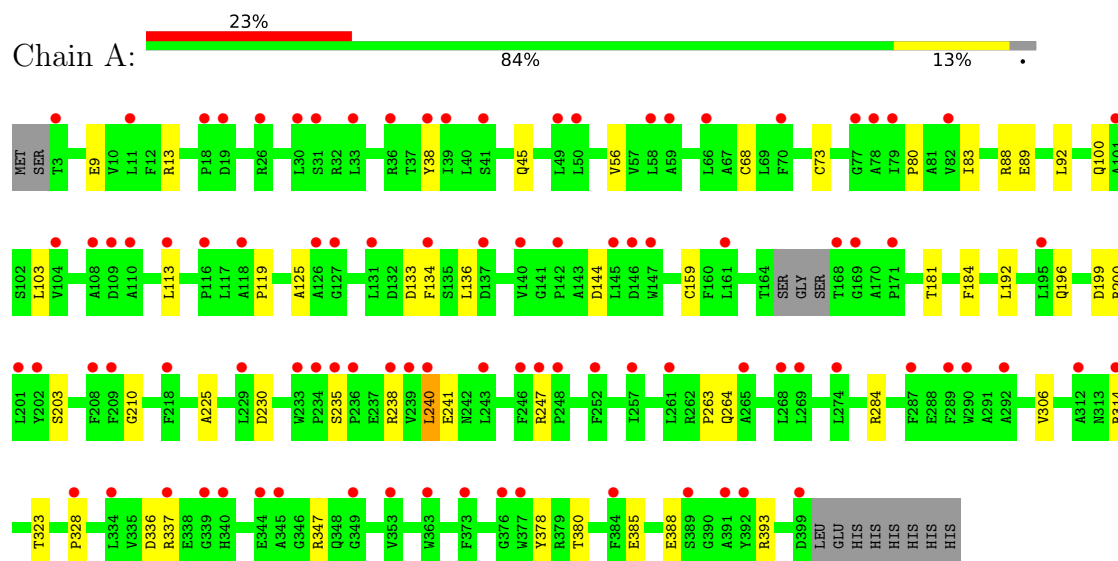
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	360	Total	O	0	2
			360	360		
4	B	388	Total	O	0	1
			388	388		
4	C	352	Total	O	0	0
			352	352		
4	D	344	Total	O	0	0
			344	344		

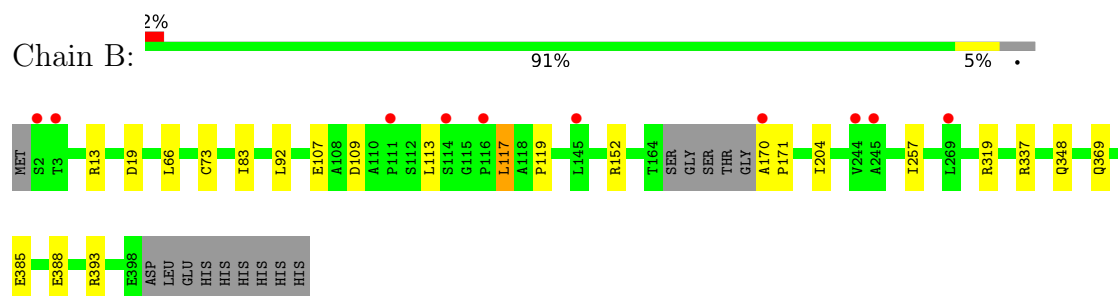
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

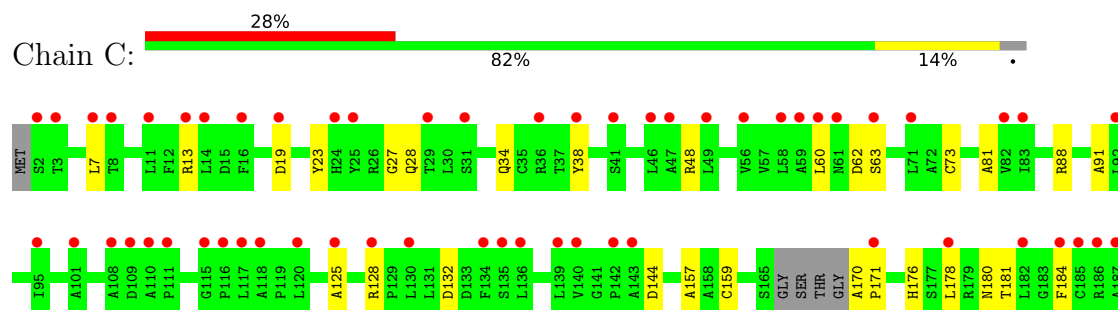
#### • Molecule 1: Anthranilate–CoA ligase

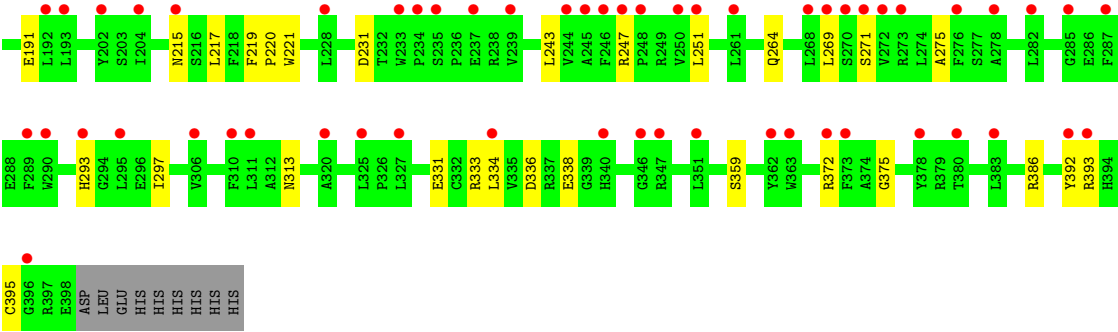


#### • Molecule 1: Anthranilate–CoA ligase

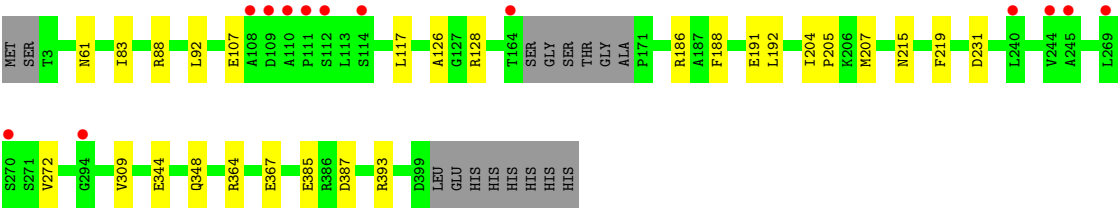
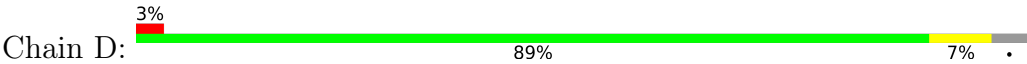


#### • Molecule 1: Anthranilate–CoA ligase





● Molecule 1: Anthranilate-CoA ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.56Å 84.13Å 138.21Å 90.00° 92.59° 90.00°	Depositor
Resolution (Å)	46.02 – 1.67 46.02 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.02-1.67) 87.2 (46.02-1.67)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.67Å)	Xtriage
Refinement program	PHENIX 1.12rc2_2821	Depositor
R, $R_{free}$	0.270 , 0.313 0.270 , 0.313	Depositor DCC
$R_{free}$ test set	9232 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.6	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.119 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	25754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1411e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 9SN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.29	0/3156	0.50	0/4292
1	B	0.34	0/3136	0.55	0/4262
1	C	0.29	0/3112	0.49	0/4233
1	D	0.34	0/3096	0.56	0/4210
All	All	0.32	0/12500	0.53	0/16997

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	3056	3017	3016	47	1
1	B	3042	3012	3012	24	0
1	C	3021	2964	2964	62	1
1	D	3011	2959	2958	23	0
2	A	33	18	0	1	0
2	B	33	18	0	0	0
2	C	33	18	0	1	0
2	D	33	18	0	1	0
3	C	10	14	14	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	360	0	0	29	8
4	B	388	0	0	16	6
4	C	352	0	0	44	8
4	D	344	0	0	16	6
All	All	13716	12038	11964	160	19

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 7.

All (160) 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:D:309:VAL:O	4:D:1002:HOH:O	1.85	0.94
1:A:89:GLU:OE1	4:A:1001:HOH:O	1.85	0.94
1:D:367:GLU:O	4:D:1001:HOH:O	1.85	0.93
1:A:314:ARG:NH1	4:A:1005:HOH:O	2.04	0.91
1:D:385:GLU:OE2	1:D:393:ARG:NH1	2.05	0.89
1:B:369:GLN:NE2	4:B:1006:HOH:O	2.09	0.86
1:C:336:ASP:OD2	4:C:1001:HOH:O	1.94	0.85
1:B:13:ARG:NH1	4:B:1005:HOH:O	2.09	0.84
1:D:387:ASP:OD2	4:D:1003:HOH:O	1.93	0.84
1:A:347:ARG:NH1	4:A:1009:HOH:O	2.10	0.83
1:C:393:ARG:NH2	4:C:1011:HOH:O	2.10	0.83
1:C:333:ARG:NE	4:C:1013:HOH:O	2.12	0.83
1:C:331:GLU:OE2	4:C:1002:HOH:O	1.97	0.82
1:B:348:GLN:NE2	4:B:1004:HOH:O	2.06	0.82
1:B:107:GLU:OE1	4:B:1002:HOH:O	1.98	0.82
1:A:133:ASP:OD1	4:A:1002:HOH:O	1.96	0.82
1:A:125:ALA:O	4:A:1003:HOH:O	1.99	0.79
1:C:372:ARG:NH1	4:C:1017:HOH:O	2.15	0.79
1:A:203:SER:O	4:A:1004:HOH:O	2.01	0.79
1:D:393:ARG:NH1	4:D:1007:HOH:O	2.16	0.78
1:C:128:ARG:NE	1:C:231:ASP:OD2	2.17	0.77
1:C:338:GLU:N	4:C:1018:HOH:O	2.16	0.77
1:C:191:GLU:OE1	4:C:1003:HOH:O	2.03	0.76
1:B:109:ASP:O	4:B:1003:HOH:O	2.03	0.76
1:A:88:ARG:NH2	4:A:1014:HOH:O	2.18	0.76
1:A:100:GLN:OE1	4:A:1006:HOH:O	2.04	0.76
1:C:62:ASP:O	4:C:1006:HOH:O	2.04	0.76
1:C:375:GLY:O	4:C:1004:HOH:O	2.03	0.75
1:C:231:ASP:OD2	4:C:1007:HOH:O	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLN:NE2	4:A:1015:HOH:O	2.20	0.73
1:D:348:GLN:OE1	4:D:1004:HOH:O	2.05	0.73
1:C:313:ASN:OD1	4:C:1009:HOH:O	2.08	0.72
1:C:125:ALA:O	4:C:1005:HOH:O	2.07	0.72
1:C:27:GLY:O	4:C:1008:HOH:O	2.07	0.71
1:C:159[B]:CYS:SG	4:C:1019:HOH:O	2.32	0.71
1:D:192:LEU:O	4:D:1005:HOH:O	2.08	0.71
1:B:113:LEU:N	4:B:1001:HOH:O	2.18	0.70
1:C:264:GLN:OE1	4:C:1010:HOH:O	2.09	0.70
1:D:191:GLU:OE1	4:D:1006:HOH:O	2.10	0.70
1:D:186:ARG:NH1	4:D:1018:HOH:O	2.25	0.69
1:C:181:THR:OG1	4:C:1012:HOH:O	2.10	0.69
1:A:134:PHE:O	4:A:1008:HOH:O	2.10	0.69
1:A:314:ARG:NH1	4:A:1023:HOH:O	2.27	0.68
1:A:263:PRO:O	4:A:1010:HOH:O	2.10	0.67
1:A:210:GLY:N	4:A:1022[B]:HOH:O	2.27	0.67
1:C:19[A]:ASP:OD2	4:C:1014:HOH:O	2.12	0.67
1:A:45:GLN:OE1	4:A:1011:HOH:O	2.12	0.66
1:B:388:GLU:OE1	4:B:1007:HOH:O	2.13	0.66
1:A:385:GLU:OE2	1:A:393:ARG:NH2	2.28	0.66
1:B:73:CYS:SG	4:B:1330:HOH:O	2.45	0.66
1:C:19[B]:ASP:OD2	4:C:1015:HOH:O	2.13	0.65
1:C:217:LEU:O	4:C:1016:HOH:O	2.15	0.65
1:A:247:ARG:NH1	4:A:1025:HOH:O	2.29	0.65
1:C:372:ARG:NH1	4:C:1026:HOH:O	2.29	0.64
1:D:128:ARG:NE	1:D:231:ASP:OD2	2.27	0.64
1:C:128:ARG:NH2	1:C:231:ASP:OD1	2.30	0.64
1:C:7:LEU:HA	1:C:178:LEU:HD13	1.81	0.63
1:C:88:ARG:NH2	4:C:1029:HOH:O	2.31	0.62
1:D:364:ARG:NE	4:D:1024:HOH:O	2.32	0.62
1:A:119:PRO:O	4:A:1012:HOH:O	2.16	0.62
1:A:38:TYR:HD2	1:A:68[B]:CYS:HG	1.48	0.62
1:B:117:LEU:O	4:B:1009:HOH:O	2.16	0.62
1:A:388:GLU:OE1	1:A:388:GLU:N	2.32	0.61
1:B:385:GLU:OE2	1:B:393:ARG:NH1	2.34	0.60
1:A:200:ARG:NH2	4:A:1035:HOH:O	2.34	0.60
1:D:272:VAL:O	4:D:1008:HOH:O	2.17	0.60
1:A:230:ASP:OD2	1:A:238:ARG:NE	2.35	0.60
1:B:117:LEU:HD12	1:B:117:LEU:N	2.17	0.59
1:B:152[B]:ARG:NH2	4:B:1022:HOH:O	2.35	0.59
1:C:81:ALA:N	4:C:1037:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:HIS:HA	4:C:1077:HOH:O	2.03	0.58
1:A:336:ASP:OD2	4:A:1009:HOH:O	2.17	0.57
1:C:269:LEU:HD21	1:C:293:HIS:O	2.04	0.57
1:A:347:ARG:O	4:A:1013:HOH:O	2.17	0.56
1:C:247:ARG:HA	1:C:271:SER:HB2	1.87	0.55
1:C:34:GLN:NE2	4:C:1046:HOH:O	2.39	0.54
3:C:901:PGE:O4	4:C:1005:HOH:O	2.04	0.54
1:A:192:LEU:N	4:A:1044:HOH:O	2.41	0.54
1:A:238:ARG:NH1	1:A:241:GLU:OE2	2.33	0.54
1:C:359:SER:HA	4:C:1077:HOH:O	2.07	0.53
1:C:334[B]:LEU:HD11	1:C:392:TYR:HE2	1.74	0.52
1:D:207:MET:HB3	4:D:1037:HOH:O	2.08	0.52
1:D:83:ILE:HD11	1:D:92:LEU:HD13	1.92	0.51
1:C:13:ARG:NH2	4:C:1053:HOH:O	2.42	0.51
1:C:221:TRP:CZ2	4:C:1048:HOH:O	2.64	0.51
1:B:19:ASP:OD1	4:B:1011:HOH:O	2.19	0.51
1:D:126:ALA:O	4:D:1009:HOH:O	2.19	0.50
1:C:220:PRO:HB2	4:C:1016:HOH:O	2.10	0.50
1:B:83:ILE:HD11	1:B:92:LEU:HD13	1.93	0.49
1:B:119:PRO:O	4:B:1010:HOH:O	2.18	0.49
1:D:88:ARG:NH1	4:D:1042:HOH:O	2.45	0.49
1:A:263:PRO:HB2	4:A:1015:HOH:O	2.11	0.49
1:B:117:LEU:N	1:B:117:LEU:CD1	2.76	0.49
1:D:204:ILE:HB	1:D:205:PRO:HD3	1.93	0.48
1:C:23:TYR:CE2	4:C:1048:HOH:O	2.56	0.48
1:D:88:ARG:NE	4:D:1016:HOH:O	2.24	0.48
1:C:275:ALA:HB3	1:C:297:ILE:HD13	1.96	0.48
1:C:243:LEU:HD21	1:C:251:LEU:HD13	1.95	0.48
1:D:344:GLU:OE1	4:D:1010:HOH:O	2.20	0.48
1:A:83:ILE:HD11	1:A:92:LEU:HD13	1.96	0.47
1:C:73:CYS:SG	4:C:1299:HOH:O	2.49	0.47
1:C:38:TYR:OH	1:C:132:ASP:O	2.23	0.47
1:A:306:VAL:HG12	1:A:306:VAL:O	2.15	0.47
1:D:188:PHE:HB2	4:D:1002:HOH:O	2.15	0.47
1:A:56[B]:VAL:HG23	1:A:80:PRO:HA	1.98	0.46
1:A:92:LEU:HG	1:A:113:LEU:HD21	1.98	0.46
1:A:378:TYR:CE2	1:A:380:THR:HA	2.50	0.46
1:C:395:CYS:HA	4:C:1129:HOH:O	2.16	0.45
1:C:221:TRP:CE2	4:C:1048:HOH:O	2.70	0.45
1:A:38:TYR:HD2	1:A:68[B]:CYS:SG	2.38	0.45
1:A:284:ARG:NH2	4:A:1067:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:THR:HA	1:A:184:PHE:CE2	2.52	0.45
2:A:900:9SN:O14	2:A:900:9SN:N32	2.50	0.45
1:A:264:GLN:HG2	4:A:1015:HOH:O	2.16	0.45
1:A:144:ASP:O	4:A:1016:HOH:O	2.21	0.44
1:C:60:LEU:HB3	3:C:901:PGE:H2	1.99	0.44
2:C:900:9SN:N32	2:C:900:9SN:O14	2.50	0.44
1:B:113:LEU:HD12	4:B:1001:HOH:O	2.17	0.44
1:B:319:ARG:NH2	4:B:1032:HOH:O	2.49	0.44
1:A:136:LEU:HG	4:A:1008:HOH:O	2.18	0.44
1:A:56[B]:VAL:HG21	1:A:73:CYS:SG	2.58	0.44
1:C:28:GLN:NE2	4:C:1023:HOH:O	2.27	0.44
1:D:215:ASN:HA	1:D:219:PHE:CD2	2.53	0.44
1:C:215:ASN:HA	1:C:219:PHE:CD2	2.53	0.43
1:C:170:ALA:HB3	1:C:171:PRO:HD3	2.00	0.43
1:B:66:LEU:C	1:B:66:LEU:HD23	2.39	0.43
1:C:91:ALA:HB2	4:C:1029:HOH:O	2.18	0.43
1:B:204:ILE:CD1	1:B:257:ILE:HG21	2.49	0.43
1:A:196:GLN:OE1	4:A:1017:HOH:O	2.21	0.43
2:D:900:9SN:N32	2:D:900:9SN:O14	2.52	0.43
1:A:9:GLU:O	1:A:13:ARG:HG2	2.19	0.43
1:B:319:ARG:NE	4:B:1016:HOH:O	2.31	0.42
1:C:7:LEU:CA	1:C:178:LEU:HD13	2.48	0.42
1:C:63:SER:OG	3:C:901:PGE:H22	2.20	0.42
1:C:333:ARG:NH2	4:C:1065:HOH:O	2.48	0.42
1:A:323:THR:N	4:A:1007:HOH:O	2.51	0.42
1:A:199:ASP:O	1:A:225:ALA:HB1	2.20	0.41
1:A:328:PRO:HD2	4:A:1044:HOH:O	2.21	0.41
1:B:204:ILE:HD12	1:B:257:ILE:HG21	2.03	0.41
1:C:63:SER:HA	4:C:1006:HOH:O	2.19	0.41
1:C:181:THR:HA	1:C:184:PHE:CE2	2.55	0.41
1:D:61:ASN:N	1:D:107:GLU:OE1	2.35	0.41
1:B:170:ALA:N	1:B:171:PRO:CD	2.84	0.41
1:C:157:ALA:O	4:C:1019:HOH:O	2.22	0.41
1:C:144:ASP:HA	4:C:1062:HOH:O	2.20	0.41
1:B:337:ARG:NE	4:B:1037:HOH:O	2.52	0.41
1:C:338:GLU:HB2	4:C:1018:HOH:O	2.21	0.41
1:A:56[B]:VAL:HG12	1:A:103:LEU:HB3	2.03	0.41
1:C:180:ASN:ND2	4:C:1077:HOH:O	2.53	0.41
1:C:334[B]:LEU:HD11	1:C:392:TYR:CE2	2.55	0.41
1:C:338:GLU:CB	4:C:1018:HOH:O	2.68	0.41
1:A:80:PRO:HD2	1:A:159:CYS:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ARG:HG2	4:A:1212:HOH:O	2.21	0.40
1:C:128:ARG:CZ	1:C:231:ASP:OD1	2.70	0.40
1:C:333:ARG:NH1	4:C:1065:HOH:O	2.54	0.40
1:A:240:LEU:HD21	1:A:264:GLN:HB3	2.02	0.40
1:C:88:ARG:CZ	4:C:1029:HOH:O	2.67	0.40
1:D:204:ILE:N	1:D:205:PRO:CD	2.85	0.40
1:C:7:LEU:HD13	1:C:178:LEU:HD12	2.02	0.40
1:C:334[B]:LEU:HD13	1:C:386:ARG:NH1	2.36	0.40

All (19) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1028:HOH:O	4:D:1138:HOH:O[1_545]	1.75	0.45
4:B:1292:HOH:O	4:D:1214:HOH:O[2_746]	1.88	0.32
4:C:1221:HOH:O	4:C:1303:HOH:O[2_545]	1.91	0.29
4:C:1010:HOH:O	4:C:1191:HOH:O[2_545]	1.95	0.25
4:B:1268:HOH:O	4:B:1321:HOH:O[2_646]	1.96	0.24
4:B:1182:HOH:O	4:D:1024:HOH:O[1_545]	1.97	0.23
4:A:1071:HOH:O	4:A:1283:HOH:O[2_645]	1.98	0.22
4:A:1249:HOH:O	4:C:1237:HOH:O[1_545]	1.98	0.22
4:A:1010:HOH:O	4:A:1140:HOH:O[2_655]	1.99	0.21
4:A:1308:HOH:O	4:C:1328:HOH:O[2_545]	1.99	0.21
4:A:1029:HOH:O	4:A:1132:HOH:O[2_645]	2.02	0.18
4:B:1287:HOH:O	4:D:1208:HOH:O[1_545]	2.02	0.18
4:A:1301:HOH:O	4:C:1344:HOH:O[2_545]	2.05	0.15
4:C:1221:HOH:O	4:C:1314:HOH:O[2_545]	2.05	0.15
1:A:235[B]:SER:OG	1:C:48:ARG:O[2_645]	2.09	0.11
4:A:1312:HOH:O	4:C:1347:HOH:O[2_645]	2.12	0.08
4:A:1267:HOH:O	4:C:1313:HOH:O[1_545]	2.15	0.05
4:B:1302:HOH:O	4:D:1275:HOH:O[1_545]	2.18	0.02
4:D:1189:HOH:O	4:D:1221:HOH:O[2_756]	2.18	0.02

## 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	398/407 (98%)	391 (98%)	7 (2%)	0	100	100
1	B	394/407 (97%)	388 (98%)	6 (2%)	0	100	100
1	C	394/407 (97%)	388 (98%)	6 (2%)	0	100	100
1	D	390/407 (96%)	383 (98%)	7 (2%)	0	100	100
All	All	1576/1628 (97%)	1550 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	315/320 (98%)	313 (99%)	2 (1%)	86	79
1	B	312/320 (98%)	311 (100%)	1 (0%)	92	89
1	C	308/320 (96%)	308 (100%)	0	100	100
1	D	307/320 (96%)	306 (100%)	1 (0%)	92	89
All	All	1242/1280 (97%)	1238 (100%)	4 (0%)	92	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	LEU
1	A	337	ARG
1	B	117	LEU
1	D	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	264	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

5 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	9SN	A	900	-	33,36,36	0.66	0	39,54,54	0.72	1 (2%)
2	9SN	B	900	-	33,36,36	0.66	0	39,54,54	0.68	1 (2%)
3	PGE	C	901	-	9,9,9	0.27	0	8,8,8	0.47	0
2	9SN	D	900	-	33,36,36	0.61	0	39,54,54	0.72	1 (2%)
2	9SN	C	900	-	33,36,36	0.66	0	39,54,54	0.90	3 (7%)

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	9SN	A	900	-	-	4/15/35/35	0/4/4/4
2	9SN	B	900	-	-	3/15/35/35	0/4/4/4
3	PGE	C	901	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9SN	D	900	-	-	2/15/35/35	0/4/4/4
2	9SN	C	900	-	-	3/15/35/35	0/4/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	9SN	O14-C24-O26	2.97	124.52	122.13
2	A	900	9SN	C3-C2-N1	2.30	123.85	120.35
2	D	900	9SN	C3-C2-N1	2.25	123.77	120.35
2	B	900	9SN	C3-C2-N1	2.20	123.70	120.35
2	C	900	9SN	P12-O14-C24	2.11	127.69	123.04
2	C	900	9SN	C3-C2-N1	2.04	123.45	120.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	901	PGE	O2-C3-C4-O3
3	C	901	PGE	O1-C1-C2-O2
3	C	901	PGE	O3-C5-C6-O4
2	A	900	9SN	C24-O14-P12-O11
2	B	900	9SN	C24-O14-P12-O11
2	D	900	9SN	C24-O14-P12-O11
3	C	901	PGE	C3-C4-O3-C5
2	A	900	9SN	O14-C24-C25-C31
2	C	900	9SN	O26-C24-C25-C31
2	C	900	9SN	C24-O14-P12-O11
2	A	900	9SN	O26-C24-C25-C27
2	A	900	9SN	O26-C24-C25-C31
2	B	900	9SN	O26-C24-C25-C31
2	B	900	9SN	O26-C24-C25-C27
2	C	900	9SN	O26-C24-C25-C27
2	D	900	9SN	O26-C24-C25-C31

There are no ring outliers.

4 monomers are involved in 6 short contacts:

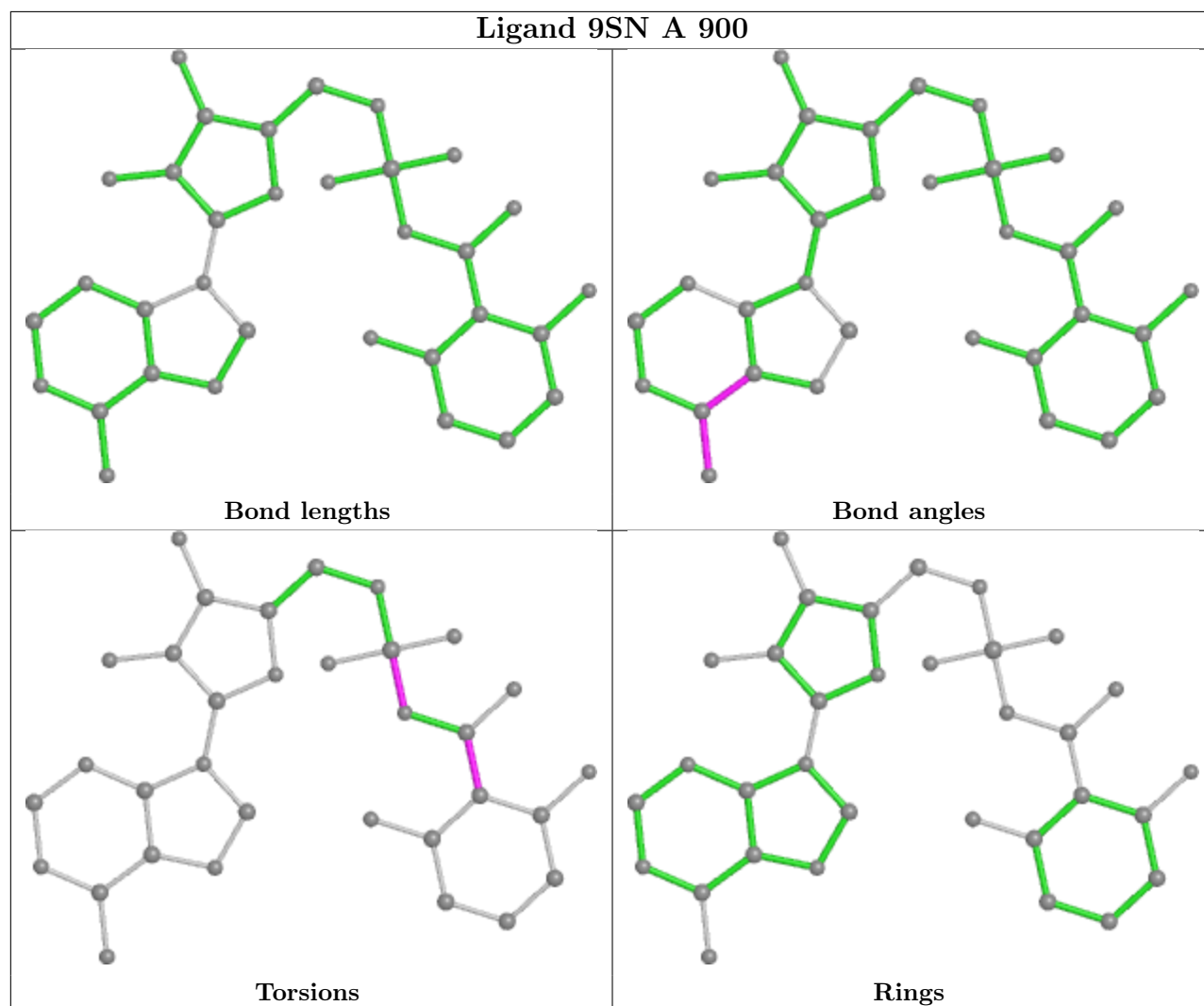
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	9SN	1	0

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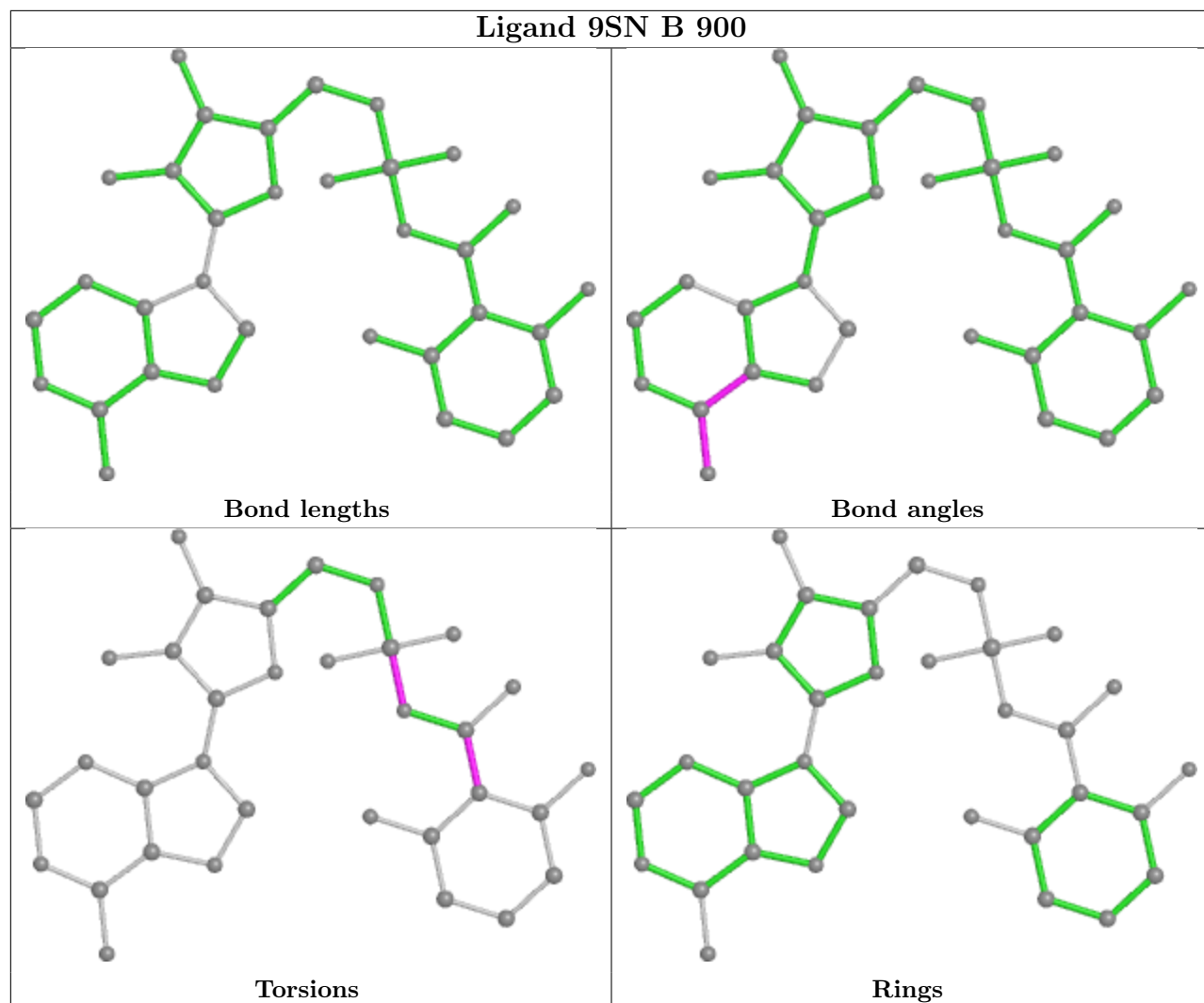
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	PGE	3	0
2	D	900	9SN	1	0
2	C	900	9SN	1	0

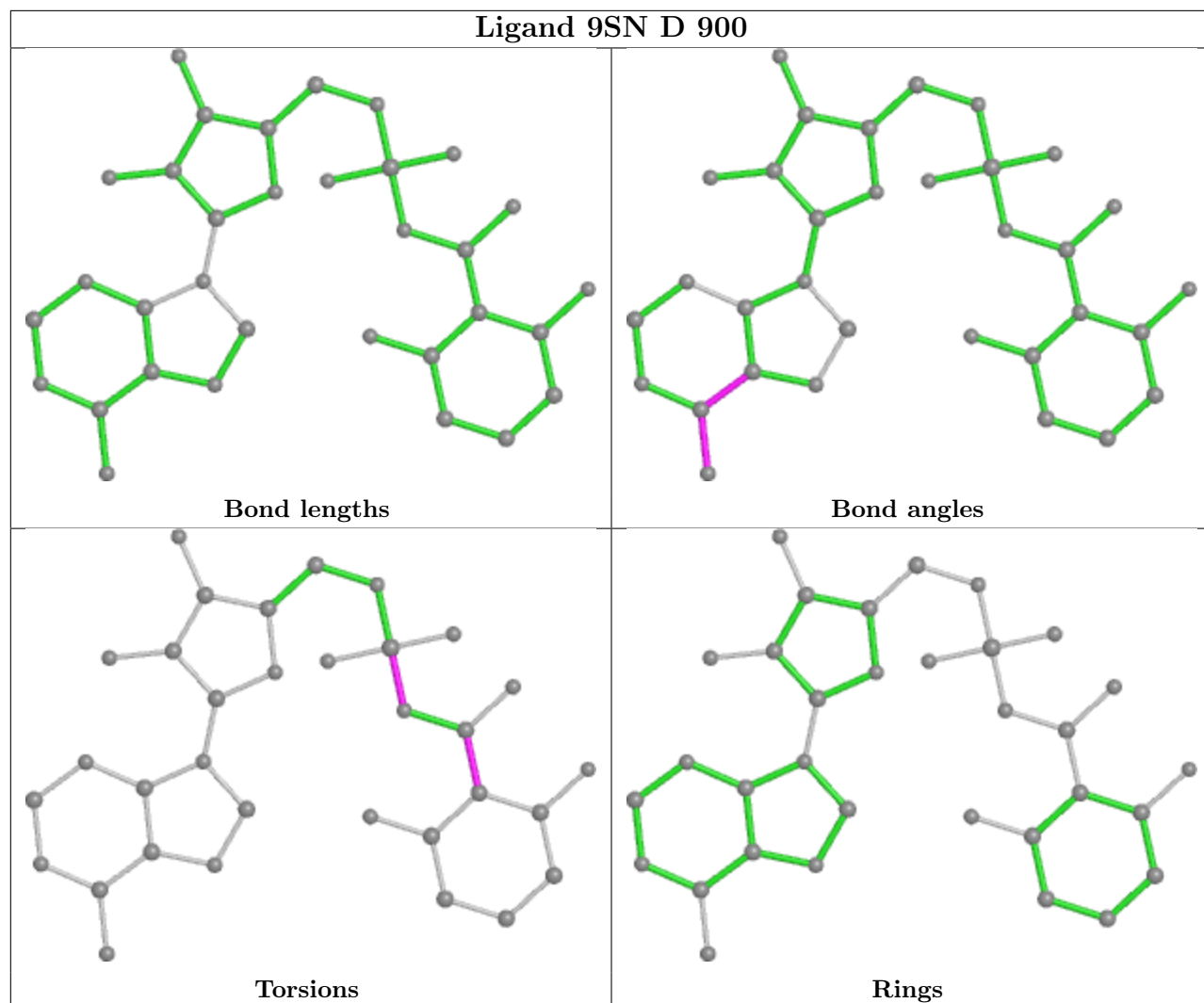
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

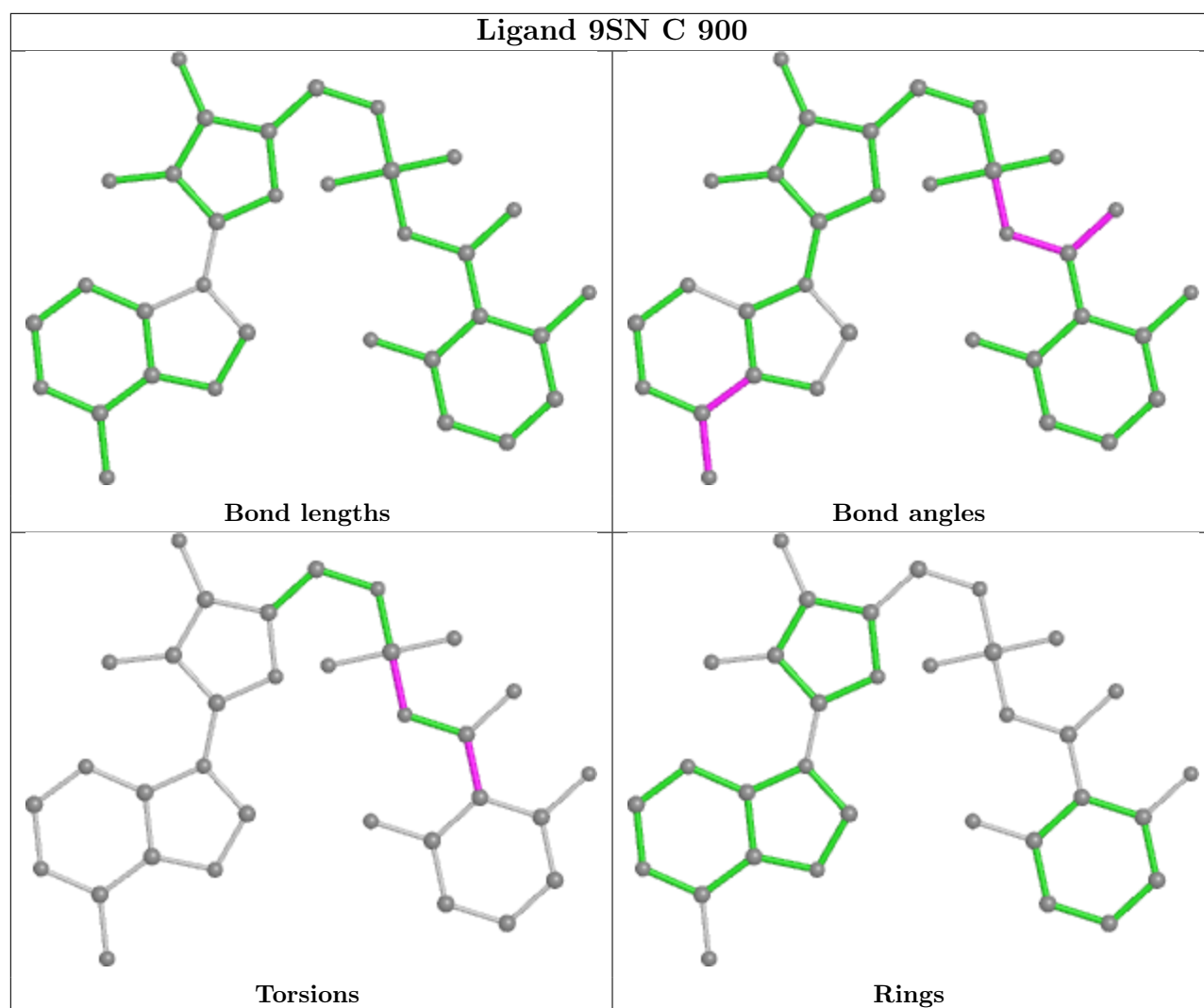


## Ligand 9SN B 900



## Ligand 9SN D 900





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	394/407 (96%)	1.44	93 (23%) <b>0</b> <b>0</b>	15, 24, 38, 54	0
1	B	392/407 (96%)	0.34	10 (2%) 56 58	3, 11, 24, 42	0
1	C	393/407 (96%)	1.59	112 (28%) <b>0</b> <b>0</b>	17, 26, 43, 57	0
1	D	391/407 (96%)	0.43	13 (3%) 46 49	3, 12, 27, 34	0
All	All	1570/1628 (96%)	0.95	228 (14%) <b>2</b> <b>2</b>	3, 21, 36, 57	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	ALA	6.5
1	A	233	TRP	5.7
1	A	209[A]	PHE	5.5
1	C	109	ASP	5.2
1	A	127	GLY	5.0
1	B	2	SER	5.0
1	A	118	ALA	4.9
1	C	268	LEU	4.9
1	C	269	LEU	4.9
1	A	3	THR	4.7
1	C	49	LEU	4.6
1	C	233	TRP	4.6
1	C	178	LEU	4.6
1	C	117	LEU	4.5
1	A	116	PRO	4.3
1	C	136	LEU	4.3
1	C	115	GLY	4.2
1	C	139	LEU	4.1
1	A	126	ALA	4.0
1	D	108	ALA	4.0
1	B	245	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	82	VAL	3.9
1	C	2	SER	3.9
1	C	271	SER	3.9
1	A	168	THR	3.9
1	A	344	GLU	3.8
1	A	363	TRP	3.8
1	C	234	PRO	3.8
1	C	61	ASN	3.8
1	C	244	VAL	3.7
1	B	170	ALA	3.6
1	A	314	ARG	3.6
1	A	202	TYR	3.6
1	A	201	LEU	3.6
1	C	311	LEU	3.6
1	A	235[A]	SER	3.6
1	C	290	TRP	3.6
1	A	50	LEU	3.6
1	B	111	PRO	3.5
1	D	164	THR	3.5
1	C	383	LEU	3.5
1	A	252	PHE	3.5
1	C	320	ALA	3.5
1	D	114	SER	3.5
1	A	131	LEU	3.5
1	C	245	ALA	3.4
1	D	110	ALA	3.3
1	A	31[A]	SER	3.3
1	C	111	PRO	3.3
1	A	110	ALA	3.3
1	A	373	PHE	3.2
1	A	274	LEU	3.2
1	C	285	GLY	3.2
1	C	47	ALA	3.2
1	A	240	LEU	3.1
1	C	373	PHE	3.1
1	C	362	TYR	3.1
1	A	146	ASP	3.1
1	A	392	TYR	3.1
1	C	171	PRO	3.0
1	C	38	TYR	3.0
1	C	108	ALA	3.0
1	A	49	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	334	LEU	3.0
1	C	192	LEU	2.9
1	C	396	GLY	2.9
1	B	114	SER	2.9
1	A	268	LEU	2.9
1	C	46	LEU	2.9
1	C	59	ALA	2.9
1	A	30	LEU	2.9
1	C	14	LEU	2.8
1	D	269	LEU	2.8
1	C	3	THR	2.8
1	C	130	LEU	2.8
1	A	246	PHE	2.8
1	C	134	PHE	2.8
1	C	261	LEU	2.8
1	B	3	THR	2.8
1	A	292	ALA	2.8
1	C	273	ARG	2.7
1	C	41	SER	2.7
1	C	60	LEU	2.7
1	A	38	TYR	2.7
1	C	202	TYR	2.7
1	D	240	LEU	2.7
1	C	270	SER	2.7
1	A	238	ARG	2.7
1	A	70	PHE	2.7
1	A	58	LEU	2.7
1	A	104	VAL	2.7
1	A	384	PHE	2.7
1	A	349	GLY	2.6
1	C	204	ILE	2.6
1	A	243	LEU	2.6
1	C	29	THR	2.6
1	C	378	TYR	2.6
1	A	345	ALA	2.6
1	D	109	ASP	2.6
1	A	257	ILE	2.6
1	A	140	VAL	2.6
1	A	108	ALA	2.6
1	C	287	PHE	2.6
1	B	269	LEU	2.6
1	C	251	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	186	ARG	2.5
1	C	184	PHE	2.5
1	C	289	PHE	2.5
1	A	312	ALA	2.5
1	A	142	PRO	2.5
1	A	218	PHE	2.5
1	C	272	VAL	2.5
1	C	7	LEU	2.5
1	A	287	PHE	2.5
1	C	276	PHE	2.5
1	A	147	TRP	2.5
1	C	8	THR	2.5
1	D	244	VAL	2.5
1	C	58	LEU	2.5
1	C	282	LEU	2.5
1	C	237	GLU	2.5
1	A	265	ALA	2.5
1	C	393	ARG	2.5
1	A	18	PRO	2.4
1	C	101	ALA	2.4
1	C	278	ALA	2.4
1	A	389	SER	2.4
1	C	13	ARG	2.4
1	A	234	PRO	2.4
1	A	236	PRO	2.4
1	C	239	VAL	2.4
1	C	92	LEU	2.4
1	C	295	LEU	2.4
1	A	399	ASP	2.4
1	D	245	ALA	2.4
1	A	137	ASP	2.4
1	C	306	VAL	2.4
1	C	228	LEU	2.4
1	C	363	TRP	2.4
1	A	26	ARG	2.4
1	C	140	VAL	2.4
1	A	134	PHE	2.4
1	A	171	PRO	2.4
1	A	36[A]	ARG	2.4
1	C	63	SER	2.4
1	C	246	PHE	2.3
1	C	25	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	392	TYR	2.3
1	A	169	GLY	2.3
1	C	187	ALA	2.3
1	A	248	PRO	2.3
1	C	193	LEU	2.3
1	C	185	CYS	2.3
1	A	247	ARG	2.3
1	C	347	ARG	2.3
1	C	24	HIS	2.3
1	C	380	THR	2.3
1	A	328	PRO	2.3
1	A	261	LEU	2.3
1	C	351	LEU	2.3
1	A	19	ASP	2.3
1	C	143	ALA	2.3
1	C	346	GLY	2.3
1	A	239	VAL	2.3
1	C	182	LEU	2.3
1	C	248	PRO	2.2
1	A	145	LEU	2.2
1	A	290	TRP	2.2
1	C	327	LEU	2.2
1	C	95	ILE	2.2
1	C	340	HIS	2.2
1	C	372	ARG	2.2
1	A	41	SER	2.2
1	C	116	PRO	2.2
1	C	142	PRO	2.2
1	C	325	LEU	2.2
1	C	36	ARG	2.2
1	C	247	ARG	2.2
1	A	11	LEU	2.2
1	A	66	LEU	2.2
1	A	229	LEU	2.2
1	D	111	PRO	2.2
1	C	215	ASN	2.2
1	C	250	VAL	2.2
1	A	269	LEU	2.2
1	A	39	ILE	2.2
1	A	376	GLY	2.2
1	A	377	TRP	2.2
1	D	294	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	82	VAL	2.1
1	A	195	LEU	2.1
1	C	135	SER	2.1
1	A	101	ALA	2.1
1	C	19[A]	ASP	2.1
1	A	339	GLY	2.1
1	A	289	PHE	2.1
1	A	59	ALA	2.1
1	A	78	ALA	2.1
1	A	113	LEU	2.1
1	A	391	ALA	2.1
1	B	145	LEU	2.1
1	C	11	LEU	2.1
1	A	109	ASP	2.1
1	D	112	SER	2.1
1	C	110	ALA	2.1
1	A	79	ILE	2.1
1	C	293	HIS	2.1
1	A	337	ARG	2.0
1	C	128	ARG	2.0
1	A	353	VAL	2.0
1	B	244	VAL	2.0
1	C	310	PHE	2.0
1	A	33	LEU	2.0
1	C	31	SER	2.0
1	C	71	LEU	2.0
1	C	334[A]	LEU	2.0
1	C	83	ILE	2.0
1	C	125	ALA	2.0
1	A	340	HIS	2.0
1	C	235	SER	2.0
1	D	270	SER	2.0
1	C	56	VAL	2.0
1	A	161	LEU	2.0
1	A	208	PHE	2.0
1	C	16	PHE	2.0
1	C	120	LEU	2.0
1	A	77	GLY	2.0
1	B	116	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

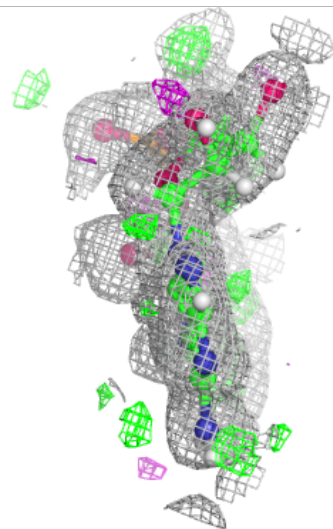
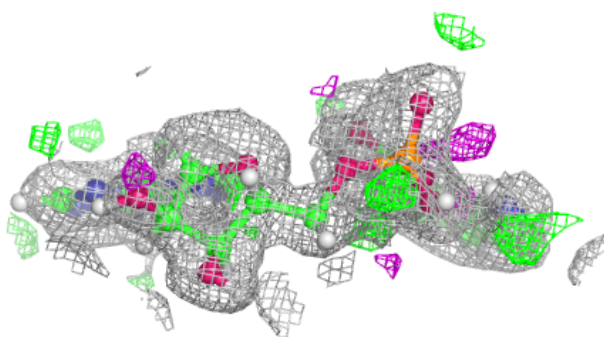
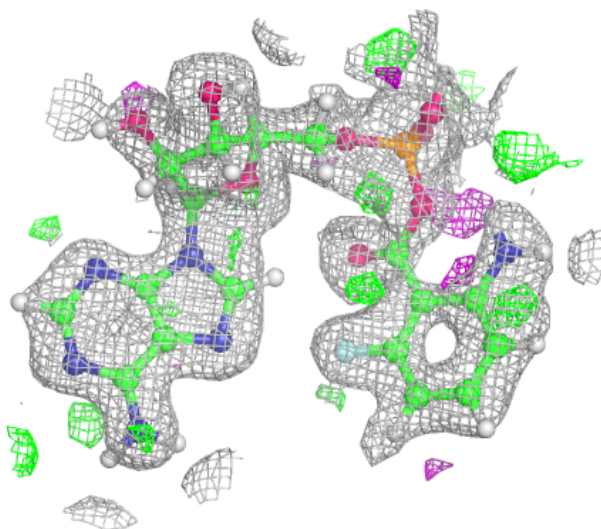
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PGE	C	901	10/10	0.83	0.21	23,35,42,50	0
2	9SN	C	900	33/33	0.87	0.13	5,15,24,34	0
2	9SN	A	900	33/33	0.93	0.11	8,19,25,28	0
2	9SN	D	900	33/33	0.94	0.11	8,8,11,23	0
2	9SN	B	900	33/33	0.96	0.09	8,8,10,13	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.

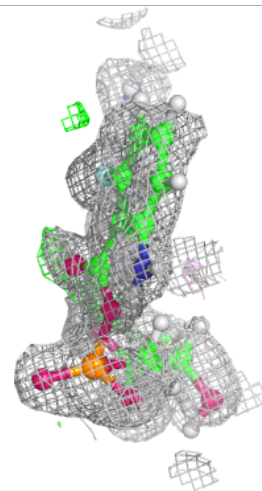
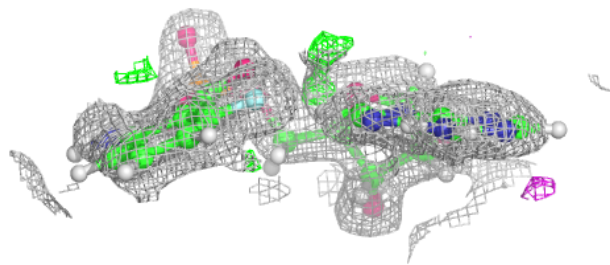
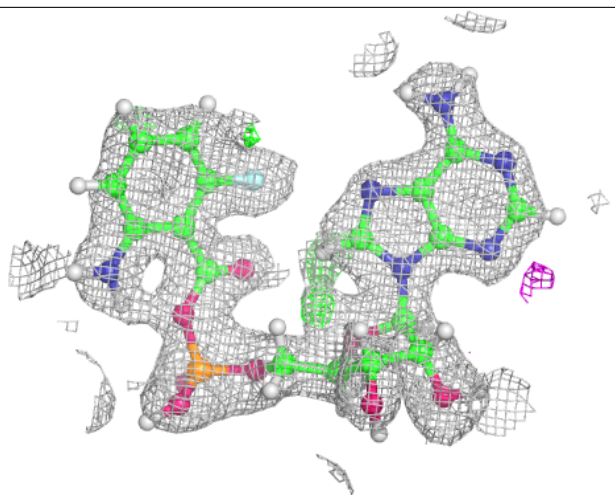
**Electron density around 9SN C 900:**

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



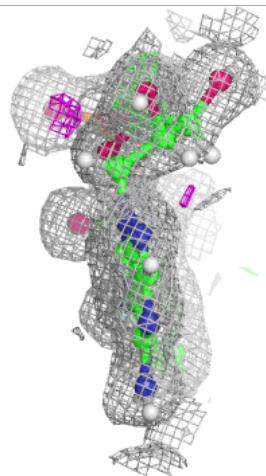
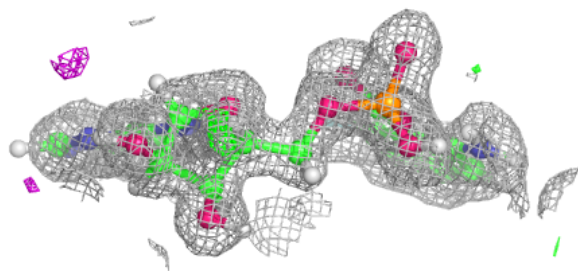
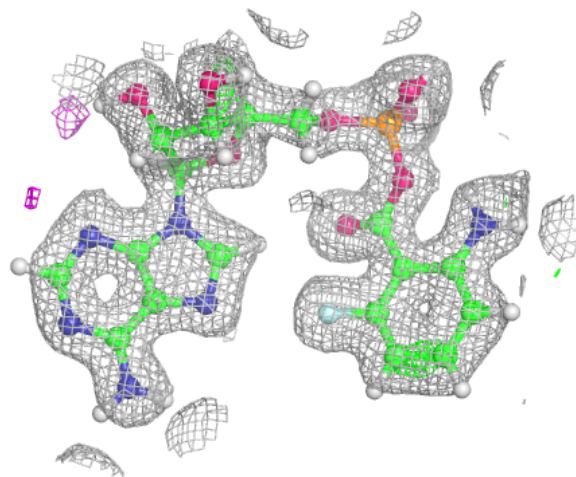
**Electron density around 9SN A 900:**

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



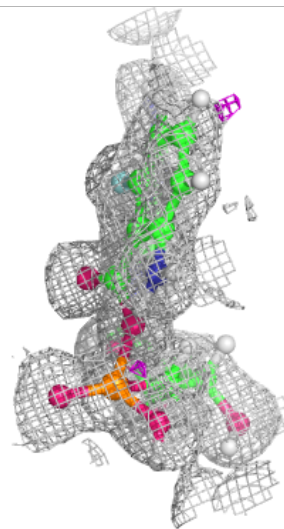
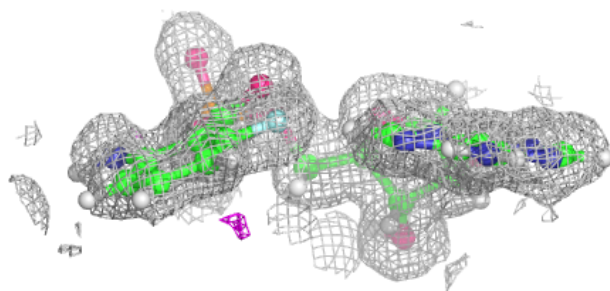
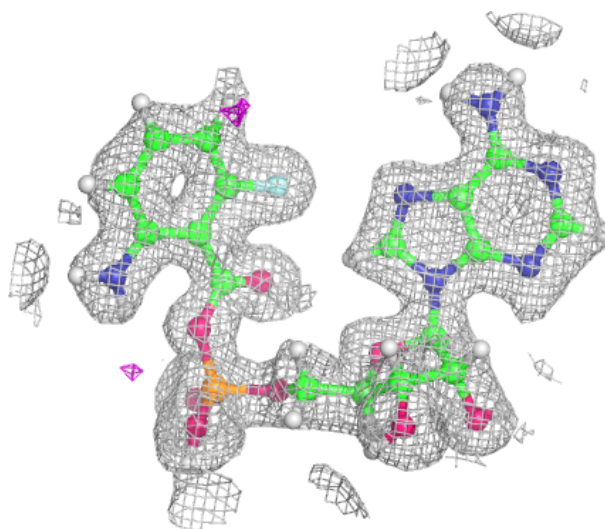
**Electron density around 9SN D 900:**

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



**Electron density around 9SN B 900:**

$2mF_o-DF_c$  (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.