



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:05 PM UTC

PDB ID : 2CLO / pdb_00002clo
Title : Tryptophan Synthase (external aldimine state) in complex with (naphthalene-2'-sulfonyl)-2-amino-1-ethylphosphate (F19)
Authors : Ngo, H.; Kimmich, N.; Harris, R.; Niks, D.; Blumenstein, L.; Kulik, V.; Barends, T.R.; Schlichting, I.; Dunn, M.F.
Deposited on : 2006-04-28
Resolution : 1.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

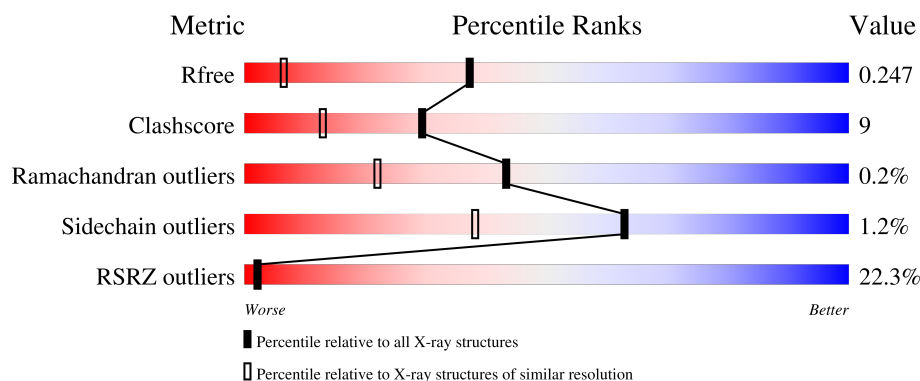
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	268	29% 71% 23% • •
2	B	396	17% 83% 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
4	PLS	B	1392	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5508 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	1
			1941	1233	338	363	7			

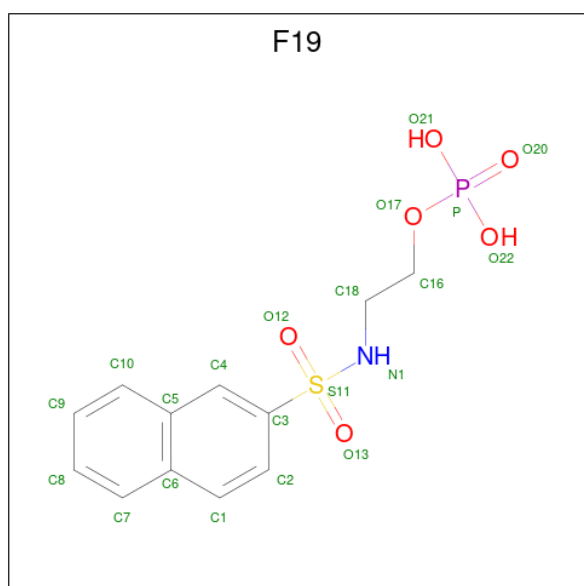
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	391	Total	C	N	O	S	0	0	1
			2954	1857	519	559	19			

There is a discrepancy between the modelled and reference sequences:

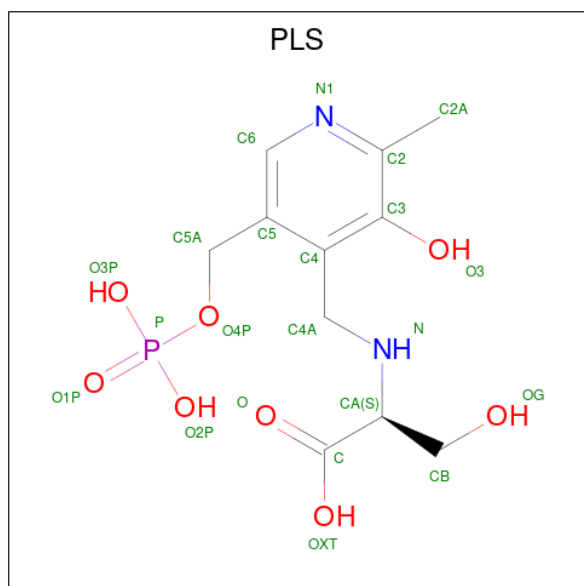
Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ARG	SER	conflict	UNP P0A2K1

- Molecule 3 is 2-[(2-NAPHTHYLSULFONYL)AMINO]ETHYL DIHYDROGEN PHOSPHATE (CCD ID: F19) (formula: $C_{12}H_{14}NO_6PS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	
			21	12	1	6	1	1	
								0	0

- Molecule 4 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (CCD ID: PLS) (formula: $C_{11}H_{17}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P		
			22	11	2	8	1		
								0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na		
			1 1	0	0

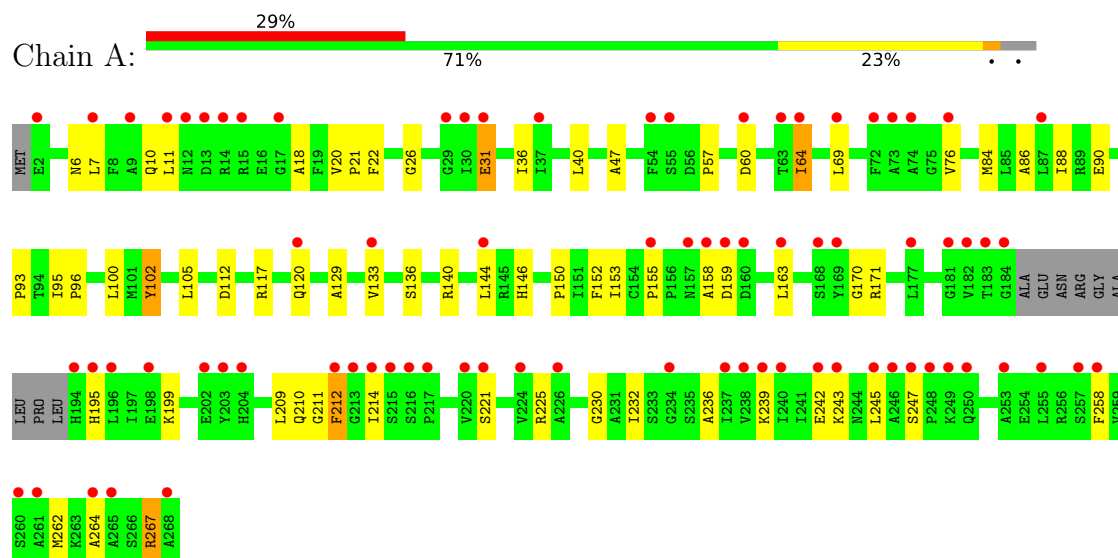
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	190	Total O		
			190 190	0	0
6	B	379	Total O		
			379 379	0	0

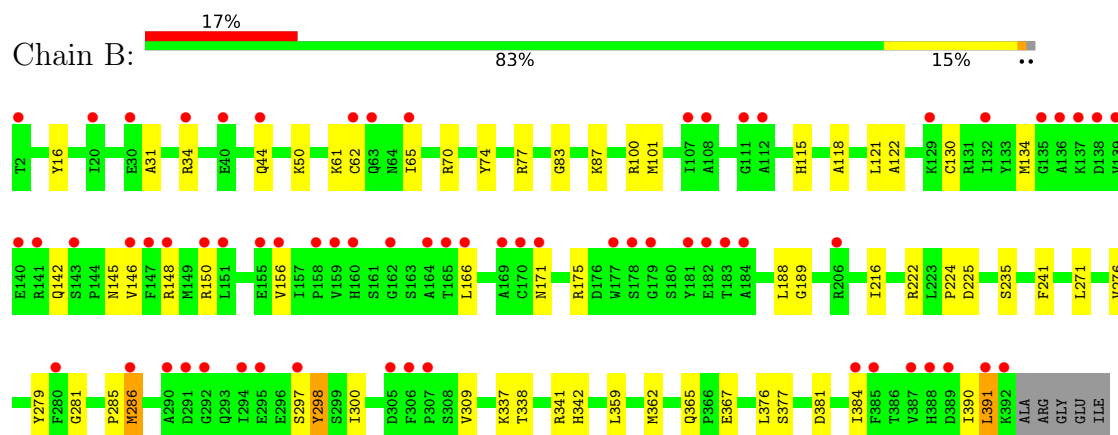
3 Residue-property plots [i](#)

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: TRYPTOPHAN SYNTHASE ALPHA CHAIN



• Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.73Å 60.14Å 67.51Å 90.00° 94.61° 90.00°	Depositor
Resolution (Å)	19.93 – 1.50 19.93 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.93-1.50) 96.4 (19.93-1.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 1.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.249 0.229 , 0.247	Depositor DCC
R_{free} test set	6217 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5508	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F19, PLS, NA

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	0.37	1/1979 (0.1%)	0.86	6/2688 (0.2%)
2	B	0.41	1/3012 (0.0%)	0.88	9/4071 (0.2%)
All	All	0.39	2/4991 (0.0%)	0.88	15/6759 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	ARG	C-N	-5.67	1.25	1.33
2	B	391	LEU	C-N	-5.63	1.25	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	77	ARG	N-CA-C	7.25	121.94	110.70
1	A	136	SER	N-CA-C	6.67	120.67	112.54
2	B	241	PHE	N-CA-C	5.67	117.53	111.36
2	B	235	SER	N-CA-C	5.63	117.22	111.14
2	B	365	GLN	CA-C-N	5.60	125.27	119.56
2	B	365	GLN	C-N-CA	5.60	125.27	119.56
1	A	93	PRO	N-CA-C	5.58	120.84	113.86
1	A	129	ALA	N-CA-C	5.41	117.87	111.33
1	A	102	TYR	N-CA-C	-5.25	101.14	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	341	ARG	N-CA-C	5.22	117.87	111.82
1	A	247	SER	CA-C-N	5.18	124.63	119.24
1	A	247	SER	C-N-CA	5.18	124.63	119.24
2	B	130	CYS	N-CA-C	5.17	116.95	108.52
2	B	377	SER	N-CA-C	5.05	117.52	111.71
2	B	166	LEU	N-CA-C	5.01	117.12	111.11

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	298	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1941	0	1943	47	0
2	B	2954	0	2927	38	0
3	A	21	0	12	1	0
4	B	22	0	13	1	0
5	B	1	0	0	0	0
6	A	190	0	0	4	0
6	B	379	0	0	11	0
All	All	5508	0	4895	85	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 9.

All (85) 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)
2:B:134:MET:HE1	6:B:2182:HOH:O	1.81	0.80
2:B:34:ARG:HB2	6:B:2139:HOH:O	1.82	0.80
1:A:211:GLY:O	1:A:212:PHE:HB2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:MET:SD	6:A:2158:HOH:O	2.47	0.72
1:A:140:ARG:O	1:A:144:LEU:HD13	1.88	0.72
1:A:150:PRO:HD2	1:A:171:ARG:HB2	1.77	0.67
2:B:44:GLN:HG3	6:B:2074:HOH:O	1.96	0.66
1:A:258:PHE:CZ	6:A:2158:HOH:O	2.50	0.64
1:A:153:ILE:HG13	3:A:1268:F19:H9	1.81	0.62
1:A:86:ALA:O	1:A:90:GLU:HG3	2.01	0.61
1:A:117:ARG:NH1	1:A:120:GLN:NE2	2.49	0.60
2:B:367:GLU:HG3	6:B:2354:HOH:O	2.03	0.59
2:B:34:ARG:HG3	2:B:100:ARG:HE	1.68	0.58
1:A:242:GLU:HA	1:A:245:LEU:HD21	1.86	0.58
1:A:20:VAL:HG22	1:A:47:ALA:HB3	1.85	0.57
1:A:155:PRO:HG2	1:A:158:ALA:HB2	1.84	0.57
2:B:279:TYR:HB3	2:B:286:MET:HE1	1.86	0.57
1:A:170:GLY:O	1:A:171:ARG:HD2	2.05	0.56
1:A:209:LEU:HD23	1:A:230:GLY:C	2.30	0.55
1:A:100:LEU:C	1:A:100:LEU:HD13	2.32	0.55
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.42	0.55
2:B:300:ILE:HD11	2:B:390:ILE:HD11	1.88	0.55
2:B:337:LYS:HD3	2:B:391:LEU:HD11	1.90	0.54
1:A:195:HIS:O	1:A:199:LYS:HG3	2.07	0.53
2:B:216:ILE:HG21	2:B:224:PRO:HD3	1.91	0.51
1:A:236:ALA:HB1	1:A:258:PHE:CZ	2.45	0.51
1:A:236:ALA:HB1	1:A:258:PHE:HZ	1.74	0.51
2:B:62:CYS:HB3	2:B:65:ILE:HG22	1.93	0.50
1:A:31:GLU:OE2	1:A:31:GLU:N	2.44	0.50
1:A:239:LYS:O	1:A:243:LYS:HG2	2.11	0.50
2:B:150:ARG:NH1	2:B:156:VAL:HB	2.27	0.49
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.94	0.49
2:B:145:ASN:ND2	2:B:148:ARG:HH21	2.11	0.49
2:B:87:LYS:CE	4:B:1392:PLS:H4A1	2.41	0.49
1:A:159:ASP:O	1:A:163:LEU:HD13	2.12	0.49
2:B:285:PRO:HG2	2:B:309:VAL:HG12	1.95	0.49
1:A:210:GLN:NE2	1:A:214:ILE:HD11	2.28	0.48
1:A:245:LEU:HD23	6:A:2172:HOH:O	2.12	0.48
2:B:16:TYR:O	2:B:281:GLY:HA2	2.13	0.48
1:A:22:PHE:CD1	1:A:22:PHE:C	2.91	0.48
1:A:60:ASP:HB3	1:A:64:ILE:HB	1.95	0.48
1:A:84:MET:O	1:A:88:ILE:HG13	2.13	0.48
2:B:142:GLN:O	2:B:146:VAL:HG23	2.14	0.48
1:A:6:ASN:O	1:A:10:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:LEU:HD12	2:B:122:ALA:N	2.29	0.47
1:A:69:LEU:HD13	6:B:2201:HOH:O	2.14	0.47
1:A:133:VAL:HG12	1:A:152:PHE:HD1	1.80	0.47
1:A:258:PHE:CE1	6:A:2158:HOH:O	2.68	0.47
1:A:264:ALA:HA	1:A:267:ARG:NH1	2.29	0.47
2:B:70:ARG:HG2	2:B:70:ARG:HH11	1.79	0.47
2:B:276:VAL:HA	2:B:285:PRO:HA	1.97	0.46
2:B:101:MET:HG2	6:B:2058:HOH:O	2.14	0.46
2:B:150:ARG:HH12	2:B:156:VAL:HB	1.81	0.46
1:A:221:SER:OG	1:A:225:ARG:NH1	2.48	0.46
1:A:36:ILE:O	1:A:40:LEU:HD13	2.16	0.46
2:B:61:LYS:HB2	2:B:74:TYR:CE1	2.50	0.45
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.98	0.45
1:A:21:PRO:HD2	1:A:47:ALA:O	2.17	0.45
2:B:83:GLY:N	6:B:2126:HOH:O	2.50	0.45
2:B:222:ARG:HH22	2:B:225:ASP:CG	2.25	0.44
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.52	0.44
2:B:285:PRO:HG2	2:B:309:VAL:CG1	2.48	0.44
1:A:117:ARG:HH11	1:A:120:GLN:CD	2.26	0.44
1:A:245:LEU:H	1:A:245:LEU:HD22	1.83	0.44
2:B:298:TYR:N	6:B:2295:HOH:O	2.50	0.44
2:B:31:ALA:HA	2:B:34:ARG:HG2	2.00	0.43
2:B:297:SER:C	6:B:2295:HOH:O	2.61	0.43
1:A:11:LEU:CD1	1:A:18:ALA:HB2	2.48	0.43
1:A:31:GLU:OE2	1:A:31:GLU:CA	2.66	0.43
1:A:242:GLU:O	1:A:245:LEU:CD2	2.66	0.43
2:B:171:ASN:O	2:B:175:ARG:HG3	2.19	0.43
2:B:31:ALA:O	2:B:34:ARG:HG2	2.19	0.43
2:B:338:THR:HG23	2:B:342:HIS:HD2	1.85	0.42
1:A:7:LEU:HD22	1:A:96:PRO:HG2	2.02	0.41
1:A:60:ASP:CG	1:A:64:ILE:HG21	2.45	0.41
2:B:381:ASP:O	2:B:384:ILE:HG12	2.21	0.41
1:A:210:GLN:HE21	1:A:214:ILE:HD11	1.86	0.41
1:A:20:VAL:HB	1:A:232:ILE:HG12	2.03	0.41
2:B:376:LEU:HD12	2:B:376:LEU:HA	1.93	0.41
2:B:118:ALA:O	2:B:121:LEU:HG	2.21	0.40
2:B:271:LEU:HD23	2:B:271:LEU:C	2.46	0.40
2:B:362:MET:HE3	6:B:2043:HOH:O	2.21	0.40
1:A:95:ILE:HA	1:A:96:PRO:HD3	1.97	0.40
2:B:50:LYS:HG3	6:B:2091:HOH:O	2.21	0.40
1:A:20:VAL:O	1:A:232:ILE:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/268 (95%)	247 (97%)	6 (2%)	1 (0%)	30	12
2	B	389/396 (98%)	377 (97%)	12 (3%)	0	100	100
All	All	643/664 (97%)	624 (97%)	18 (3%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/208 (97%)	198 (98%)	3 (2%)	57	31
2	B	305/310 (98%)	302 (99%)	3 (1%)	68	45
All	All	506/518 (98%)	500 (99%)	6 (1%)	63	38

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	64	ILE

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Mol	Chain	Res	Type
1	A	105	LEU
2	B	188	LEU
2	B	286	MET
2	B	359	LEU

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	10	GLN
1	A	120	GLN
1	A	146	HIS
1	A	147	ASN
1	A	165	GLN
1	A	210	GLN
1	A	250	GLN
2	B	26	ASN
2	B	27	GLN
2	B	36	GLN
2	B	44	GLN
2	B	64	ASN
2	B	142	GLN
2	B	145	ASN
2	B	171	ASN
2	B	236	ASN
2	B	375	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	F19	A	1268	-	22,22,22	3.31	10 (45%)	31,32,32	2.50	8 (25%)
4	PLS	B	1392	-	22,22,22	5.28	14 (63%)	28,31,31	2.83	12 (42%)

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
3	F19	A	1268	-	-	5/15/15/15	0/2/2/2
4	PLS	B	1392	-	-	4/17/17/17	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1392	PLS	C3-C2	13.00	1.54	1.41
3	A	1268	F19	C8-C7	10.32	1.58	1.36
4	B	1392	PLS	C3-C4	9.75	1.54	1.40
4	B	1392	PLS	O-C	8.22	1.46	1.22
4	B	1392	PLS	C6-C5	8.16	1.53	1.37
4	B	1392	PLS	C2A-C2	-8.07	1.37	1.50
3	A	1268	F19	S11-N1	5.60	1.70	1.61
4	B	1392	PLS	P-O4P	-5.58	1.42	1.60
4	B	1392	PLS	C4A-N	-4.53	1.33	1.46
3	A	1268	F19	C9-C10	4.50	1.46	1.36
3	A	1268	F19	C2-C3	4.35	1.45	1.38
4	B	1392	PLS	C2-N1	4.30	1.41	1.33
4	B	1392	PLS	C5-C4	4.01	1.46	1.40
4	B	1392	PLS	CA-C	3.78	1.62	1.52
4	B	1392	PLS	CB-CA	-3.59	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1392	PLS	P-O3P	-3.56	1.41	1.54
3	A	1268	F19	P-O22	-3.54	1.41	1.54
3	A	1268	F19	C3-S11	3.42	1.81	1.76
4	B	1392	PLS	P-O2P	-2.88	1.44	1.54
4	B	1392	PLS	C6-N1	2.76	1.40	1.34
3	A	1268	F19	P-O21	-2.66	1.44	1.54
3	A	1268	F19	C4-C3	2.29	1.41	1.36
3	A	1268	F19	C9-C8	2.29	1.43	1.38
3	A	1268	F19	O12-S11	2.25	1.46	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1392	PLS	C4A-N-CA	8.01	128.87	113.84
3	A	1268	F19	C8-C9-C10	-7.79	109.97	120.40
4	B	1392	PLS	O3P-P-O4P	7.12	125.24	106.67
3	A	1268	F19	O22-P-O17	5.72	121.57	106.67
3	A	1268	F19	C8-C7-C6	-5.58	112.73	120.48
3	A	1268	F19	O13-S11-O12	-5.21	113.19	119.52
4	B	1392	PLS	O4P-C5A-C5	4.29	117.40	109.36
4	B	1392	PLS	O3-C3-C2	3.89	125.65	117.58
4	B	1392	PLS	C6-N1-C2	3.86	126.20	119.20
3	A	1268	F19	C3-S11-N1	3.45	112.31	107.54
4	B	1392	PLS	OXT-C-O	-2.96	117.36	124.08
4	B	1392	PLS	C5-C6-N1	-2.91	119.09	123.83
3	A	1268	F19	O12-S11-N1	2.73	111.28	107.03
4	B	1392	PLS	OXT-C-CA	2.69	122.60	113.51
3	A	1268	F19	C2-C3-C4	-2.51	117.71	121.14
4	B	1392	PLS	CB-CA-N	2.47	116.25	109.05
4	B	1392	PLS	C4A-C4-C5	-2.36	117.18	119.75
3	A	1268	F19	C4-C3-S11	2.28	121.97	120.07
4	B	1392	PLS	C3-C2-N1	-2.27	118.10	120.96
4	B	1392	PLS	C4A-C4-C3	2.17	122.87	119.98

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1392	PLS	CB-CA-N-C4A
4	B	1392	PLS	C5-C4-C4A-N
3	A	1268	F19	C18-N1-S11-O12
4	B	1392	PLS	C3-C4-C4A-N

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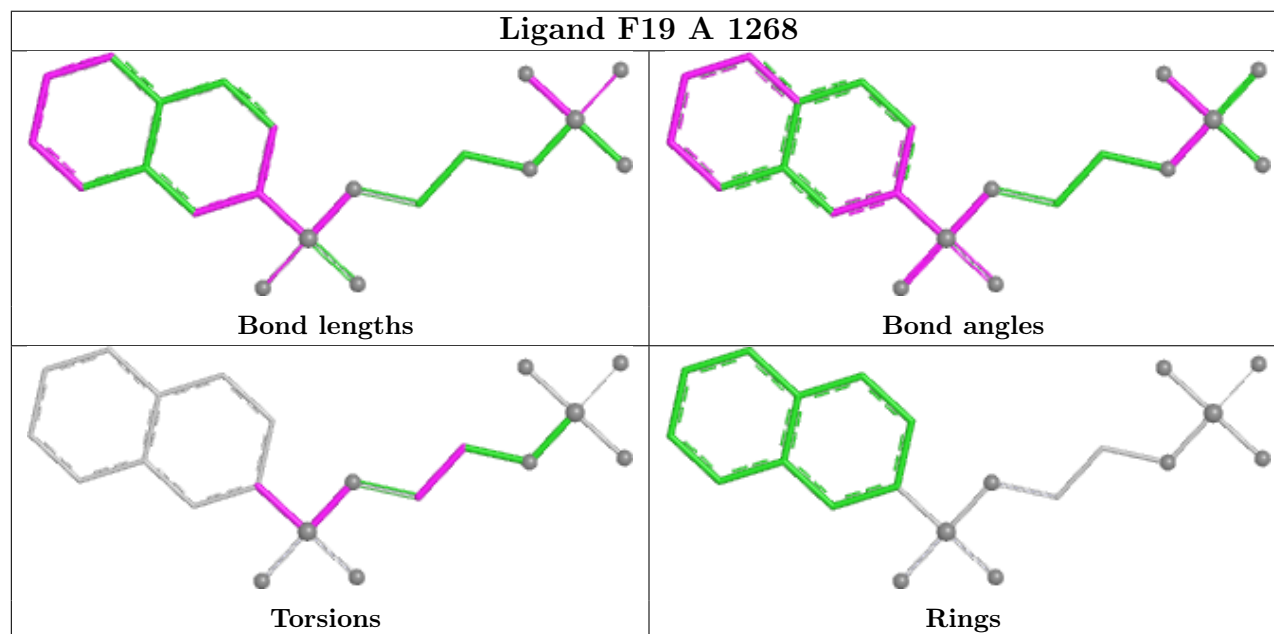
Mol	Chain	Res	Type	Atoms
4	B	1392	PLS	C-CA-N-C4A
3	A	1268	F19	C2-C3-S11-O13
3	A	1268	F19	C4-C3-S11-O13
3	A	1268	F19	C18-N1-S11-C3
3	A	1268	F19	O17-C16-C18-N1

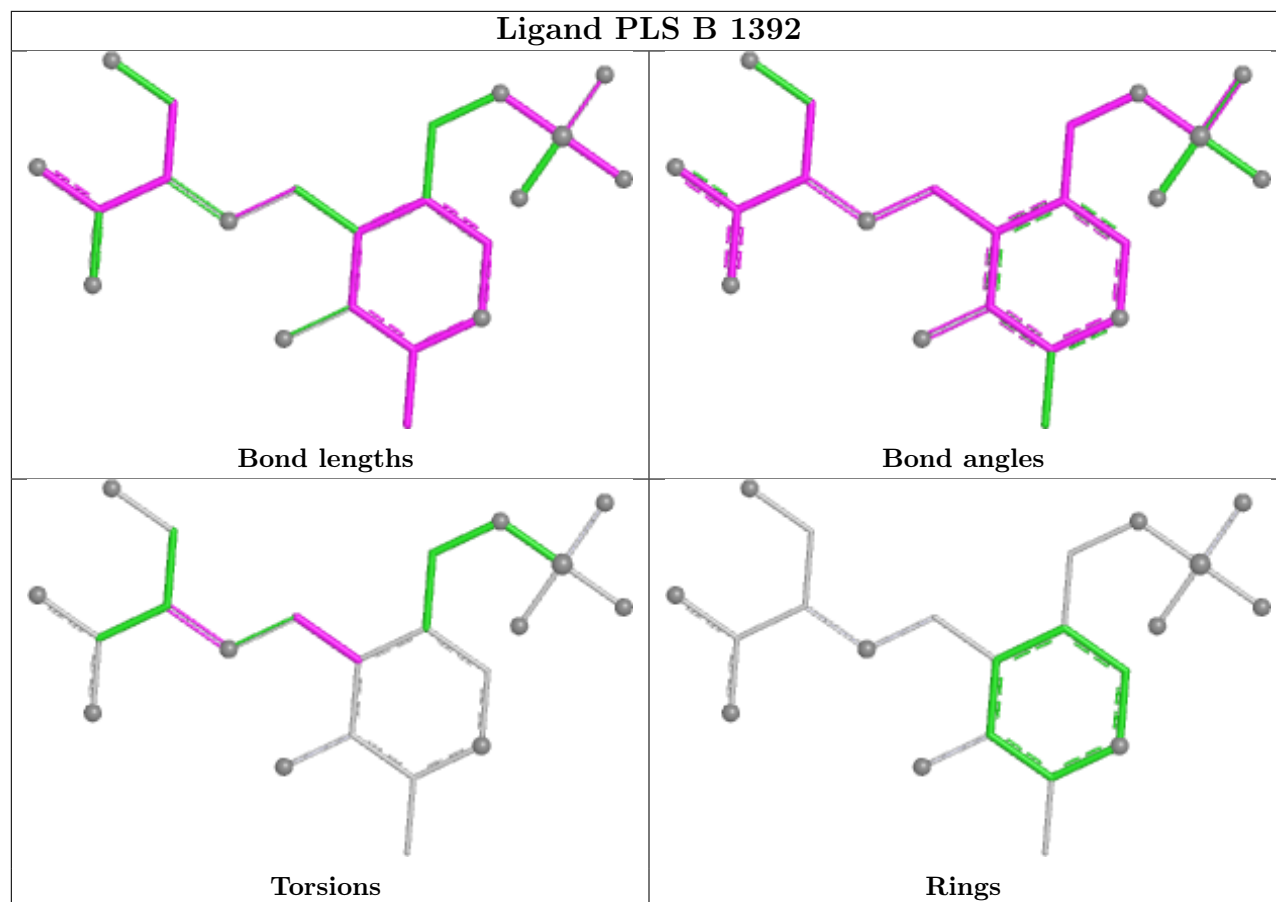
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1268	F19	1	0
4	B	1392	PLS	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.





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	258/268 (96%)	1.57	79 (30%) 1 1	10, 22, 30, 33	0
2	B	391/396 (98%)	0.62	66 (16%) 4 4	8, 14, 26, 35	0
All	All	649/664 (97%)	1.00	145 (22%) 2 2	8, 18, 29, 35	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	HIS	5.1
2	B	181	TYR	4.9
2	B	385	PHE	4.8
2	B	135	GLY	4.7
2	B	178	SER	4.7
2	B	147	PHE	4.6
2	B	384	ILE	4.6
2	B	164	ALA	4.5
2	B	140	GLU	4.4
1	A	195	HIS	4.3
2	B	63	GLN	4.3
2	B	305	ASP	4.2
1	A	239	LYS	4.1
2	B	297	SER	4.1
1	A	183	THR	3.9
2	B	62	CYS	3.8
2	B	182	GLU	3.7
2	B	2	THR	3.7
1	A	212	PHE	3.7
1	A	157	ASN	3.7
1	A	246	ALA	3.7
1	A	224	VAL	3.7
1	A	198	GLU	3.7
1	A	181	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	213	GLY	3.7
1	A	264	ALA	3.6
1	A	182	VAL	3.6
2	B	146	VAL	3.6
2	B	292	GLY	3.5
1	A	177	LEU	3.5
2	B	169	ALA	3.5
2	B	139	VAL	3.5
1	A	226	ALA	3.4
2	B	150	ARG	3.4
1	A	245	LEU	3.4
2	B	65	ILE	3.3
2	B	141	ARG	3.3
1	A	69	LEU	3.3
1	A	184	GLY	3.3
1	A	268	ALA	3.2
2	B	290	ALA	3.2
1	A	221	SER	3.2
1	A	217	PRO	3.2
2	B	171	ASN	3.1
1	A	247	SER	3.1
2	B	143	SER	3.1
1	A	258	PHE	3.1
2	B	166	LEU	3.0
2	B	391	LEU	3.0
1	A	17	GLY	3.0
1	A	29	GLY	3.0
1	A	73	ALA	3.0
1	A	74	ALA	3.0
1	A	253	ALA	3.0
2	B	307	PRO	3.0
2	B	162	GLY	3.0
1	A	196	LEU	3.0
1	A	13	ASP	2.9
1	A	87	LEU	2.9
2	B	40	GLU	2.9
1	A	250	GLN	2.9
2	B	294	ILE	2.9
2	B	165	THR	2.9
1	A	72	PHE	2.8
2	B	286	MET	2.8
1	A	63	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	183	THR	2.8
1	A	2	GLU	2.8
1	A	7	LEU	2.8
1	A	158	ALA	2.8
2	B	392	LYS	2.8
2	B	280	PHE	2.7
1	A	249	LYS	2.7
1	A	257	SER	2.7
2	B	155	GLU	2.7
1	A	9	ALA	2.7
1	A	243	LYS	2.7
1	A	240	ILE	2.7
1	A	54	PHE	2.7
1	A	261	ALA	2.6
2	B	136	ALA	2.6
1	A	204	HIS	2.6
2	B	306	PHE	2.6
1	A	260	SER	2.6
1	A	214	ILE	2.6
1	A	30	ILE	2.5
2	B	148	ARG	2.5
1	A	238	VAL	2.5
2	B	159	VAL	2.5
2	B	107	ILE	2.5
2	B	34	ARG	2.5
2	B	388	HIS	2.5
2	B	111	GLY	2.5
1	A	220	VAL	2.5
2	B	129	LYS	2.5
1	A	120	GLN	2.5
2	B	44	GLN	2.5
1	A	242	GLU	2.4
2	B	137	LYS	2.4
2	B	156	VAL	2.4
1	A	60	ASP	2.4
1	A	203	TYR	2.4
2	B	177	TRP	2.4
2	B	151	LEU	2.4
2	B	184	ALA	2.3
1	A	159	ASP	2.3
2	B	158	PRO	2.3
1	A	64	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	265	ALA	2.3
2	B	389	ASP	2.3
1	A	37	ILE	2.3
1	A	144	LEU	2.3
1	A	15	ARG	2.3
2	B	206	ARG	2.3
2	B	112	ALA	2.3
1	A	168	SER	2.3
2	B	295	GLU	2.3
1	A	133	VAL	2.3
1	A	160	ASP	2.3
2	B	138	ASP	2.3
2	B	387	VAL	2.2
1	A	55	SER	2.2
1	A	163	LEU	2.2
2	B	170	CYS	2.2
1	A	234	GLY	2.2
1	A	216	SER	2.2
2	B	20	ILE	2.2
1	A	76	VAL	2.2
2	B	160	HIS	2.2
1	A	248	PRO	2.1
2	B	108	ALA	2.1
2	B	132	ILE	2.1
1	A	14	ARG	2.1
1	A	31	GLU	2.1
1	A	202	GLU	2.1
1	A	237	ILE	2.1
2	B	291	ASP	2.1
1	A	255	LEU	2.1
2	B	179	GLY	2.1
1	A	155	PRO	2.1
2	B	30	GLU	2.0
1	A	169	TYR	2.0
1	A	215	SER	2.0
1	A	12	ASN	2.0
1	A	11	LEU	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](#)

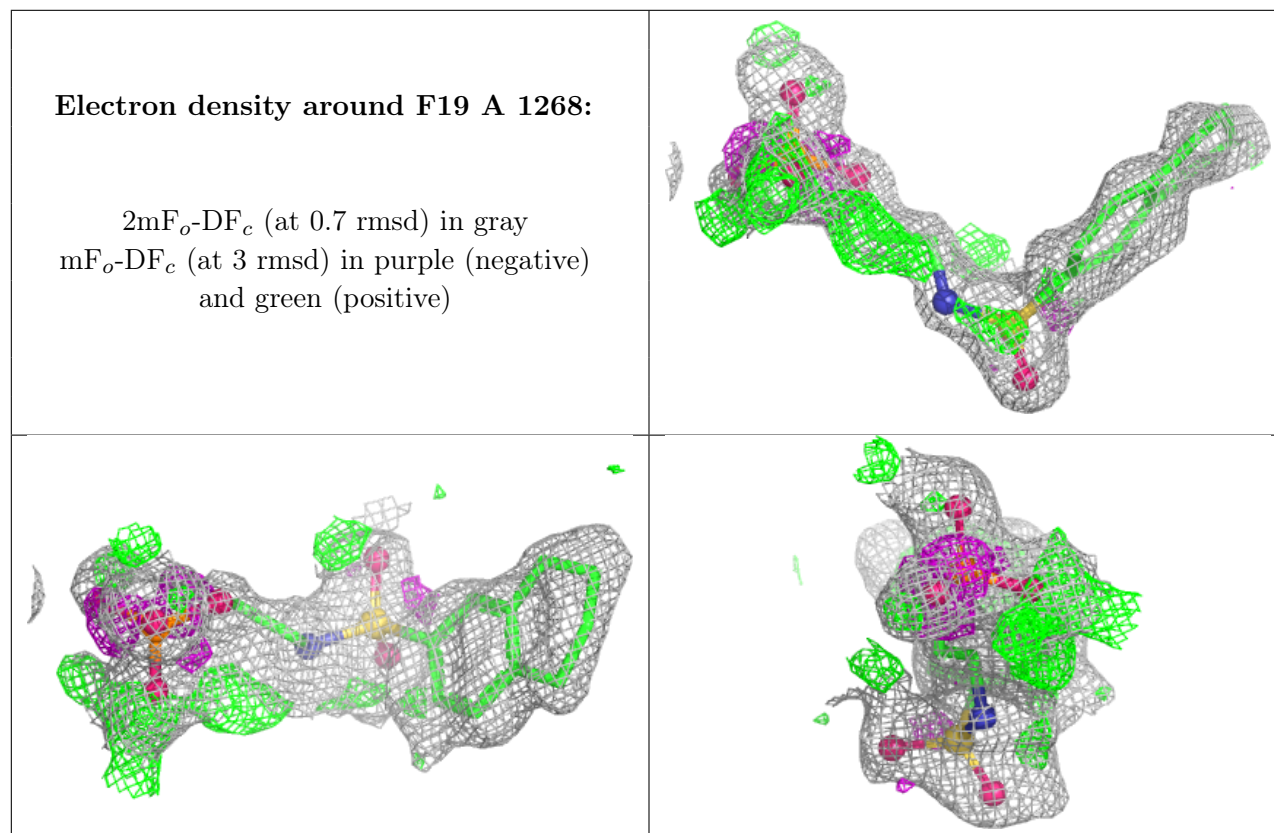
There are no oligosaccharides in this entry.

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.

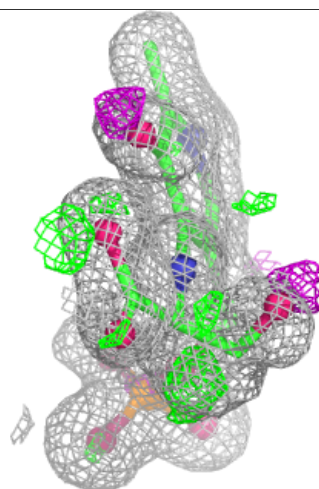
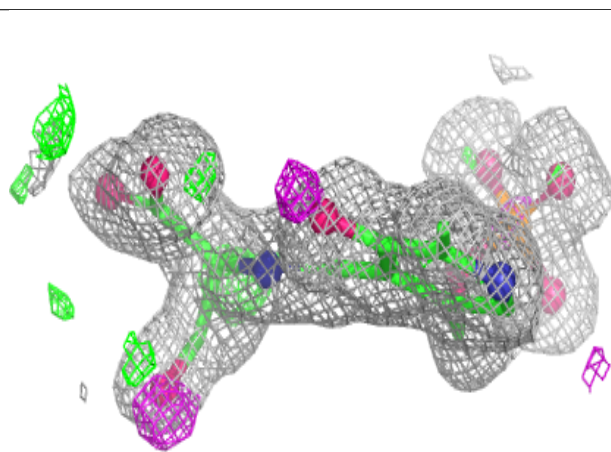
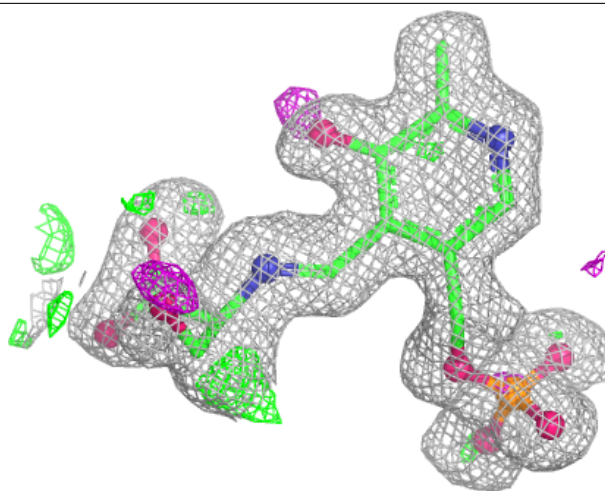
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	F19	A	1268	21/21	0.85	0.16	26,31,33,34	0
4	PLS	B	1392	22/22	0.95	0.10	7,16,23,24	0
5	NA	B	1393	1/1	0.96	0.06	14,14,14,14	0

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 PLS B 1392:

$2mF_o-DF_c$ (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.