



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:48 PM UTC

PDB ID : 2CLL / pdb_00002cll
Title : Tryptophan Synthase (external aldimine state) in complex with N-(4'- trifluoromethoxybenzenesulfonyl)-2-amino-1-ethylphosphate (F9)
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 : 1.60 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

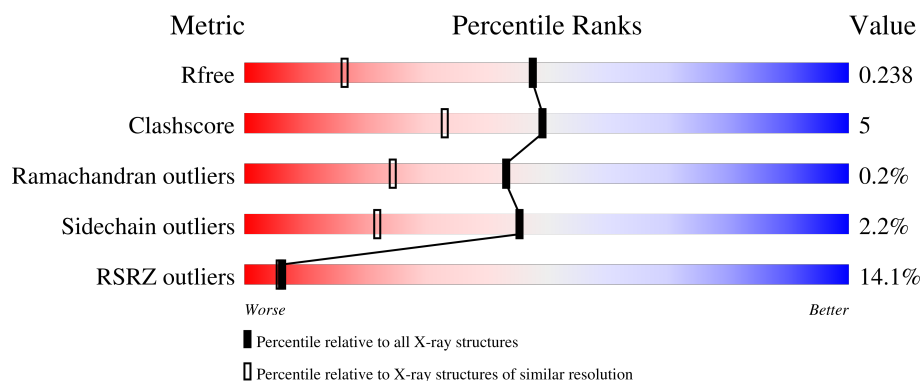
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	24% 73% 22% .
2	B	396	7% 88% 11% .

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	1395	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5425 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.

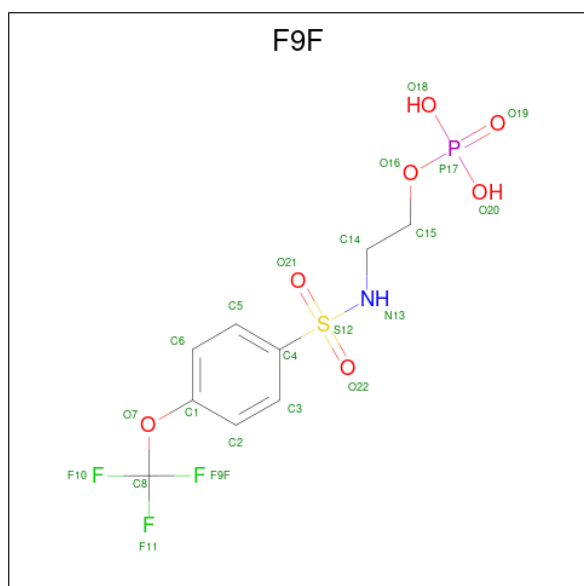
- Molecule 1 is a protein called TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	1
			1899	1206	326	360	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	0	1
			2958	1859	521	559	19			

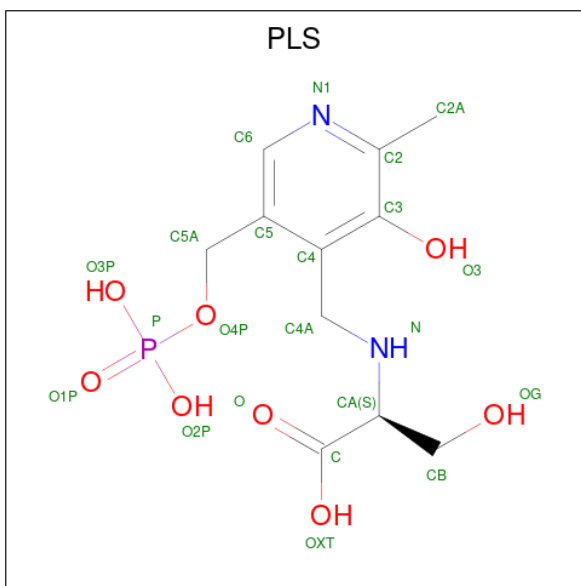
- Molecule 3 is 2-([4-(TRIFLUOROMETHOXY)PHENYL]SULFONYL)AMINO)ETHYL DIHYDROGEN PHOSPHATE (CCD ID: F9F) (formula: C₉H₁₁F₃NO₇PS).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	S	0	0
			22	9	3	1	7	1	1		

- Molecule 4 is [3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-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	0	0
			22	11	2	8	1		

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

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

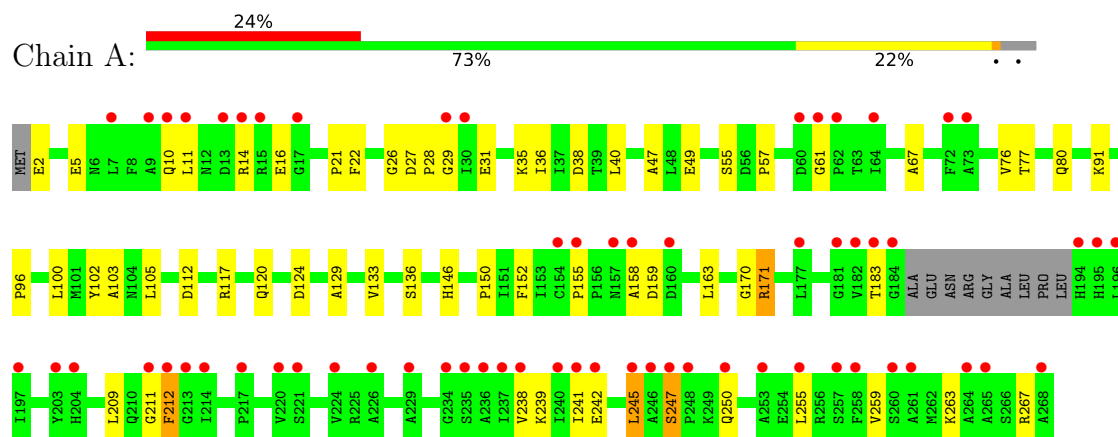
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	140	Total	O	0	0
			140	140		
6	B	383	Total	O	0	0
			383	383		

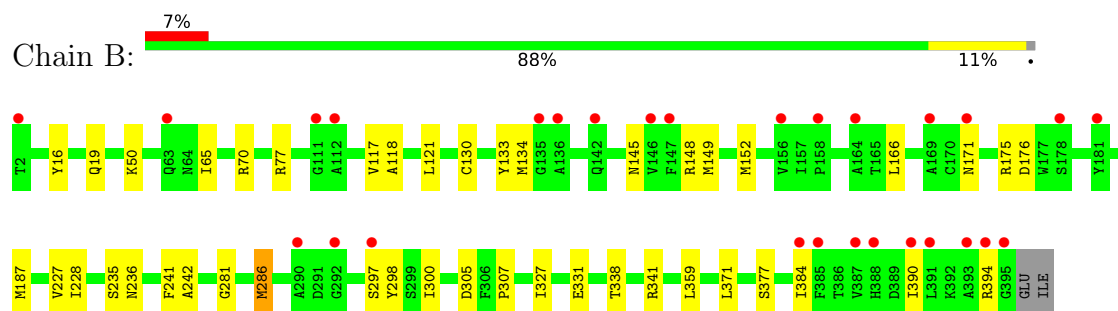
3 Residue-property plots [i](#)

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	182.53Å 59.77Å 67.34Å 90.00° 94.66° 90.00°	Depositor
Resolution (Å)	19.36 – 1.60 19.36 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (19.36-1.60) 95.7 (19.36-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.245 0.209 , 0.238	Depositor DCC
R_{free} test set	5786 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: F9F, 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	0.65	1/1935 (0.1%)	1.00	5/2636 (0.2%)
2	B	0.92	6/3016 (0.2%)	1.07	15/4079 (0.4%)
All	All	0.82	7/4951 (0.1%)	1.04	20/6715 (0.3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	70	ARG	NE-CZ	17.46	1.52	1.33
2	B	187	MET	SD-CE	-15.45	1.41	1.79
2	B	134	MET	SD-CE	7.57	1.98	1.79
2	B	394	ARG	C-N	-7.04	1.23	1.33
2	B	70	ARG	CZ-NH2	5.72	1.40	1.33
2	B	70	ARG	CD-NE	5.59	1.54	1.46
1	A	267	ARG	C-N	-5.27	1.25	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	ARG	NE-CZ-NH1	9.23	130.73	121.50
1	A	136	SER	N-CA-C	7.58	122.36	113.18
2	B	70	ARG	CD-NE-CZ	-7.02	114.58	124.40
2	B	70	ARG	NH1-CZ-NH2	-6.83	110.42	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	242	ALA	N-CA-C	6.18	118.53	111.11
2	B	241	PHE	N-CA-C	6.12	118.03	111.36
2	B	77	ARG	N-CA-C	5.81	118.33	109.62
2	B	305	ASP	N-CA-C	5.71	120.25	113.28
1	A	103	ALA	N-CA-C	5.64	118.16	111.33
2	B	130	CYS	N-CA-C	5.55	117.57	108.52
2	B	377	SER	N-CA-C	5.51	118.05	111.71
2	B	166	LEU	N-CA-C	5.47	117.95	111.33
2	B	341	ARG	N-CA-C	5.40	118.08	111.82
2	B	235	SER	N-CA-C	5.34	116.91	111.14
1	A	55	SER	N-CA-C	5.24	116.99	111.28
2	B	241	PHE	CB-CA-C	-5.20	102.01	110.85
1	A	49	GLU	N-CA-C	-5.20	99.94	108.41
2	B	384	ILE	N-CA-C	5.17	116.52	110.62
1	A	129	ALA	N-CA-C	5.07	116.80	111.28
2	B	286	MET	N-CA-C	5.02	116.82	109.24

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	1899	0	1861	36	0
2	B	2958	0	2920	17	0
3	A	22	0	9	1	0
4	B	22	0	14	0	0
5	B	1	0	0	0	0
6	A	140	0	0	4	0
6	B	383	0	0	1	0
All	All	5425	0	4804	52	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 (52) 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:211:GLY:O	1:A:212:PHE:HB2	1.88	0.73
2:B:145:ASN:HD22	2:B:148:ARG:HE	1.39	0.69
1:A:2:GLU:HB3	6:A:2080:HOH:O	1.96	0.66
1:A:100:LEU:C	1:A:100:LEU:HD13	2.21	0.65
2:B:65:ILE:HD11	2:B:338:THR:HG22	1.80	0.62
1:A:5:GLU:HG3	6:A:2005:HOH:O	2.01	0.60
1:A:31:GLU:HG2	6:A:2018:HOH:O	2.01	0.60
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.84	0.59
1:A:183:THR:HG21	3:A:1268:F9F:H5	1.84	0.58
1:A:133:VAL:HG13	2:B:19:GLN:OE1	2.06	0.56
1:A:150:PRO:HD2	1:A:171:ARG:HB2	1.88	0.56
1:A:241:ILE:O	1:A:245:LEU:HD13	2.07	0.55
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.90	0.54
1:A:11:LEU:HD22	1:A:16:GLU:HG3	1.91	0.52
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.44	0.52
1:A:36:ILE:O	1:A:40:LEU:HD13	2.10	0.52
2:B:117:VAL:HG13	2:B:152:MET:HE1	1.91	0.52
1:A:242:GLU:O	1:A:245:LEU:HD22	2.10	0.51
1:A:117:ARG:NH1	1:A:120:GLN:NE2	2.58	0.51
1:A:133:VAL:HG12	1:A:152:PHE:HD1	1.75	0.50
2:B:145:ASN:ND2	2:B:148:ARG:HE	2.09	0.49
1:A:22:PHE:C	1:A:22:PHE:CD1	2.91	0.48
1:A:155:PRO:HG2	1:A:158:ALA:HB2	1.96	0.48
1:A:21:PRO:HD2	1:A:47:ALA:O	2.14	0.48
1:A:170:GLY:O	1:A:171:ARG:HD3	2.13	0.47
1:A:133:VAL:HG12	1:A:152:PHE:CD1	2.50	0.47
1:A:61:GLY:HA3	1:A:183:THR:O	2.14	0.47
1:A:77:THR:OG1	1:A:80:GLN:HG3	2.15	0.46
1:A:239:LYS:HA	1:A:242:GLU:HG2	1.98	0.46
2:B:327:ILE:HG23	2:B:331:GLU:HB2	1.96	0.46
1:A:247:SER:HB2	1:A:250:GLN:HB3	1.97	0.45
1:A:26:GLY:O	1:A:29:GLY:N	2.50	0.45
1:A:67:ALA:HB2	1:A:238:VAL:HG11	1.99	0.44
1:A:255:LEU:O	1:A:259:VAL:HG23	2.17	0.44
2:B:133:TYR:OH	2:B:176:ASP:OD2	2.27	0.44
2:B:145:ASN:O	2:B:149:MET:HE3	2.17	0.44
2:B:65:ILE:CD1	2:B:338:THR:HG22	2.46	0.44
2:B:50:LYS:HG3	6:B:2088:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:VAL:C	2:B:228:ILE:HG13	2.43	0.43
1:A:100:LEU:C	1:A:100:LEU:CD1	2.90	0.43
2:B:171:ASN:O	2:B:175:ARG:HG3	2.19	0.43
1:A:27:ASP:HA	1:A:28:PRO:HA	1.84	0.42
1:A:263:LYS:HE2	6:A:2024:HOH:O	2.19	0.42
2:B:300:ILE:HD11	2:B:390:ILE:CD1	2.49	0.42
2:B:65:ILE:HD11	2:B:338:THR:CG2	2.49	0.42
1:A:38:ASP:OD2	1:A:91:LYS:NZ	2.46	0.42
2:B:16:TYR:O	2:B:281:GLY:HA2	2.20	0.42
2:B:297:SER:OG	2:B:307:PRO:HA	2.20	0.41
2:B:118:ALA:O	2:B:121:LEU:HG	2.20	0.41
1:A:10:GLN:HB3	1:A:14:ARG:HH12	1.86	0.41
1:A:96:PRO:HA	1:A:124:ASP:OD2	2.21	0.41
1:A:31:GLU:O	1:A:35:LYS:HG3	2.21	0.41

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%)	246 (97%)	7 (3%)	1 (0%)	30	14
2	B	392/396 (99%)	383 (98%)	9 (2%)	0	100	100
All	All	646/664 (97%)	629 (97%)	16 (2%)	1 (0%)	43	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE

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	191/208 (92%)	184 (96%)	7 (4%)	30	10
2	B	303/310 (98%)	299 (99%)	4 (1%)	61	40
All	All	494/518 (95%)	483 (98%)	11 (2%)	45	22

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	159	ASP
1	A	163	LEU
1	A	171	ARG
1	A	209	LEU
1	A	245	LEU
1	A	247	SER
2	B	236	ASN
2	B	286	MET
2	B	359	LEU
2	B	371	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	68	ASN
1	A	120	GLN
1	A	146	HIS
2	B	36	GLN
2	B	44	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	$\# Z > 2$
4	PLS	B	1395	-	22,22,22	4.45	13 (59%)	28,31,31	2.79	13 (46%)
3	F9F	A	1268	-	22,22,22	3.40	6 (27%)	32,33,33	1.64	7 (21%)

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
4	PLS	B	1395	-	-	4/17/17/17	0/1/1/1
3	F9F	A	1268	-	-	8/20/20/20	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1268	F9F	C5-C4	11.08	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1395	PLS	C3-C2	10.88	1.52	1.41
3	A	1268	F9F	S12-N13	7.68	1.73	1.61
4	B	1395	PLS	O-C	7.65	1.44	1.22
4	B	1395	PLS	C3-C4	7.18	1.50	1.40
4	B	1395	PLS	C2A-C2	-6.93	1.39	1.50
4	B	1395	PLS	C2-N1	6.25	1.44	1.33
3	A	1268	F9F	C2-C1	6.11	1.50	1.38
4	B	1395	PLS	C4A-N	-5.02	1.32	1.46
4	B	1395	PLS	CA-N	4.06	1.55	1.46
4	B	1395	PLS	C5-C4	3.92	1.46	1.40
4	B	1395	PLS	P-O4P	-3.51	1.49	1.60
4	B	1395	PLS	C6-N1	3.43	1.41	1.34
4	B	1395	PLS	CB-CA	-3.26	1.43	1.53
4	B	1395	PLS	CA-C	3.19	1.60	1.52
3	A	1268	F9F	C3-C2	3.02	1.43	1.38
4	B	1395	PLS	P-O3P	-2.23	1.46	1.54
3	A	1268	F9F	P17-O16	2.21	1.67	1.60
3	A	1268	F9F	O7-C8	2.14	1.43	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1395	PLS	C4A-N-CA	7.94	128.74	113.84
4	B	1395	PLS	O3P-P-O4P	5.53	121.08	106.67
4	B	1395	PLS	O3-C3-C2	4.83	127.60	117.58
3	A	1268	F9F	C3-C2-C1	-4.02	115.13	119.73
3	A	1268	F9F	C2-C3-C4	3.91	123.25	119.44
4	B	1395	PLS	C3-C2-N1	-3.63	116.38	120.96
4	B	1395	PLS	O4P-C5A-C5	3.54	116.00	109.36
4	B	1395	PLS	CB-CA-N	3.51	119.30	109.05
4	B	1395	PLS	C6-N1-C2	3.13	124.88	119.20
3	A	1268	F9F	C6-C1-C2	2.97	124.49	120.16
4	B	1395	PLS	C6-C5-C4	2.79	120.17	118.06
4	B	1395	PLS	OXT-C-CA	2.73	122.76	113.51
3	A	1268	F9F	O22-S12-O21	-2.68	116.26	119.52
4	B	1395	PLS	C2A-C2-C3	2.44	123.66	120.80
4	B	1395	PLS	C3-C4-C5	2.38	120.89	118.73
4	B	1395	PLS	OXT-C-O	-2.37	118.69	124.08
3	A	1268	F9F	O22-S12-C4	-2.28	105.11	107.98
3	A	1268	F9F	O21-S12-C4	-2.21	105.19	107.98
3	A	1268	F9F	O22-S12-N13	2.19	110.43	107.03
4	B	1395	PLS	C5-C6-N1	-2.12	120.38	123.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

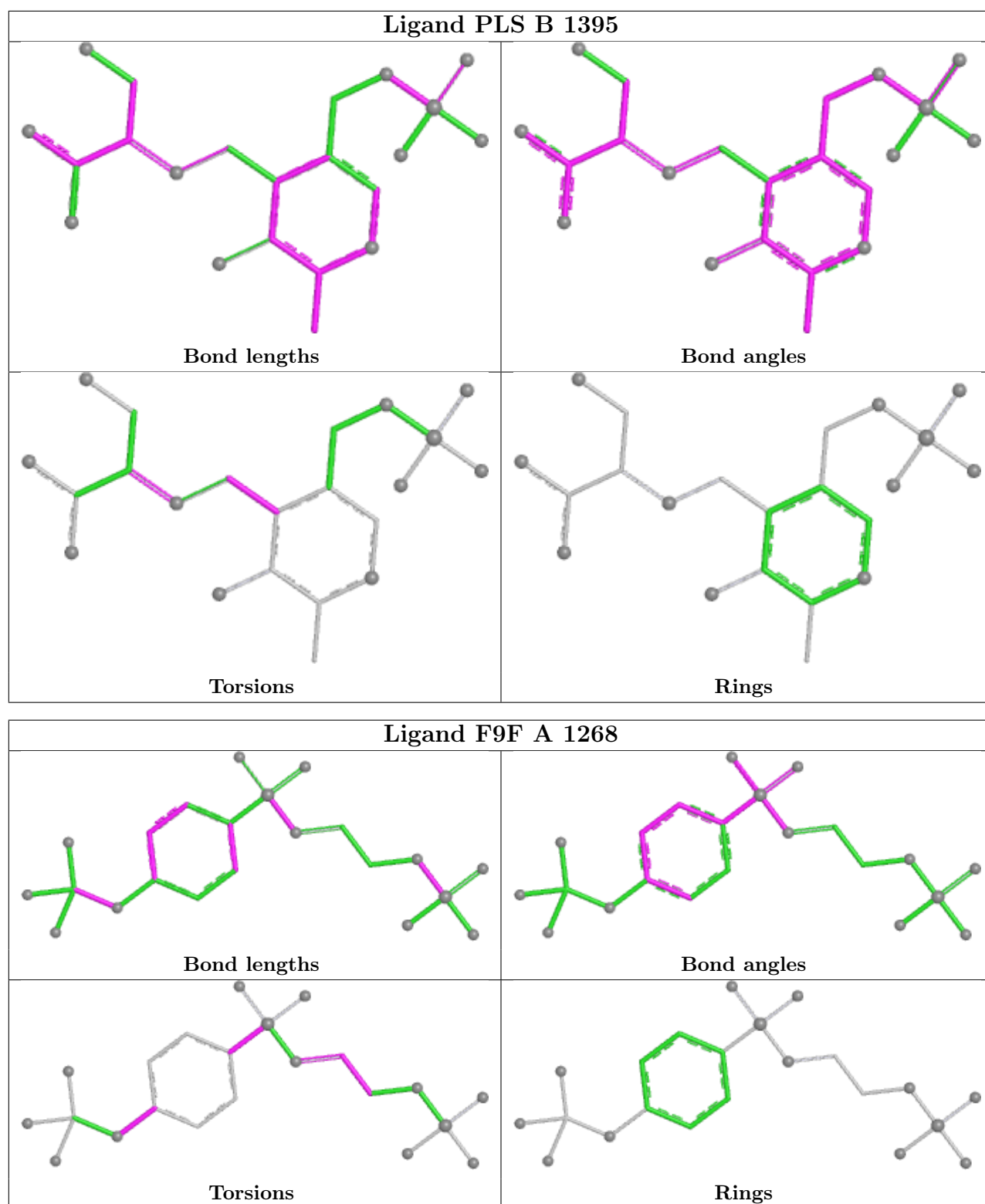
Mol	Chain	Res	Type	Atoms
4	B	1395	PLS	C-CA-N-C4A
4	B	1395	PLS	C5-C4-C4A-N
3	A	1268	F9F	C5-C4-S12-N13
3	A	1268	F9F	C3-C4-S12-N13
4	B	1395	PLS	C3-C4-C4A-N
3	A	1268	F9F	N13-C14-C15-O16
3	A	1268	F9F	C3-C4-S12-O21
3	A	1268	F9F	C5-C4-S12-O21
3	A	1268	F9F	C2-C1-O7-C8
4	B	1395	PLS	CB-CA-N-C4A
3	A	1268	F9F	C15-C14-N13-S12
3	A	1268	F9F	C6-C1-O7-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1268	F9F	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 ⓘ

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%)	1.22	64 (24%) 2 1	11, 27, 43, 67	0
2	B	394/396 (99%)	0.10	28 (7%) 22 22	7, 14, 30, 54	0
All	All	652/664 (98%)	0.54	92 (14%) 6 6	7, 19, 40, 67	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	HIS	6.8
2	B	391	LEU	5.8
1	A	268	ALA	4.4
2	B	146	VAL	4.3
2	B	181	TYR	4.2
1	A	157	ASN	4.0
1	A	247	SER	3.9
2	B	178	SER	3.9
2	B	393	ALA	3.8
1	A	183	THR	3.8
1	A	212	PHE	3.7
1	A	177	LEU	3.7
1	A	245	LEU	3.6
1	A	158	ALA	3.5
2	B	395	GLY	3.5
1	A	261	ALA	3.4
1	A	217	PRO	3.2
1	A	17	GLY	3.1
1	A	246	ALA	3.1
1	A	195	HIS	3.0
1	A	184	GLY	3.0
1	A	73	ALA	3.0
1	A	264	ALA	3.0
2	B	390	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	135	GLY	2.9
1	A	220	VAL	2.9
1	A	253	ALA	2.9
1	A	196	LEU	2.9
1	A	240	ILE	2.9
2	B	2	THR	2.8
1	A	197	ILE	2.8
1	A	248	PRO	2.8
1	A	250	GLN	2.7
2	B	290	ALA	2.7
1	A	224	VAL	2.7
1	A	242	GLU	2.7
1	A	9	ALA	2.7
2	B	164	ALA	2.7
1	A	181	GLY	2.6
1	A	182	VAL	2.6
1	A	238	VAL	2.6
2	B	136	ALA	2.6
1	A	11	LEU	2.6
2	B	297	SER	2.6
1	A	236	ALA	2.6
1	A	258	PHE	2.5
1	A	15	ARG	2.5
1	A	155	PRO	2.5
1	A	221	SER	2.5
1	A	14	ARG	2.5
1	A	241	ILE	2.5
1	A	29	GLY	2.5
2	B	171	ASN	2.5
2	B	112	ALA	2.5
1	A	234	GLY	2.5
2	B	111	GLY	2.5
2	B	384	ILE	2.5
1	A	72	PHE	2.4
1	A	213	GLY	2.4
1	A	64	ILE	2.4
1	A	60	ASP	2.4
2	B	292	GLY	2.4
1	A	226	ALA	2.4
1	A	257	SER	2.4
1	A	203	TYR	2.4
1	A	204	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	61	GLY	2.4
1	A	7	LEU	2.3
1	A	265	ALA	2.3
2	B	387	VAL	2.3
2	B	158	PRO	2.3
2	B	63	GLN	2.3
2	B	385	PHE	2.3
1	A	214	ILE	2.3
1	A	255	LEU	2.3
1	A	260	SER	2.3
1	A	235	SER	2.2
1	A	13	ASP	2.2
1	A	211	GLY	2.2
1	A	160	ASP	2.2
2	B	142	GLN	2.2
2	B	147	PHE	2.2
1	A	30	ILE	2.2
1	A	229	ALA	2.2
2	B	169	ALA	2.2
1	A	10	GLN	2.1
1	A	237	ILE	2.1
2	B	394	ARG	2.1
2	B	388	HIS	2.1
1	A	154	CYS	2.1
1	A	62	PRO	2.1
2	B	156	VAL	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 [\(i\)](#)

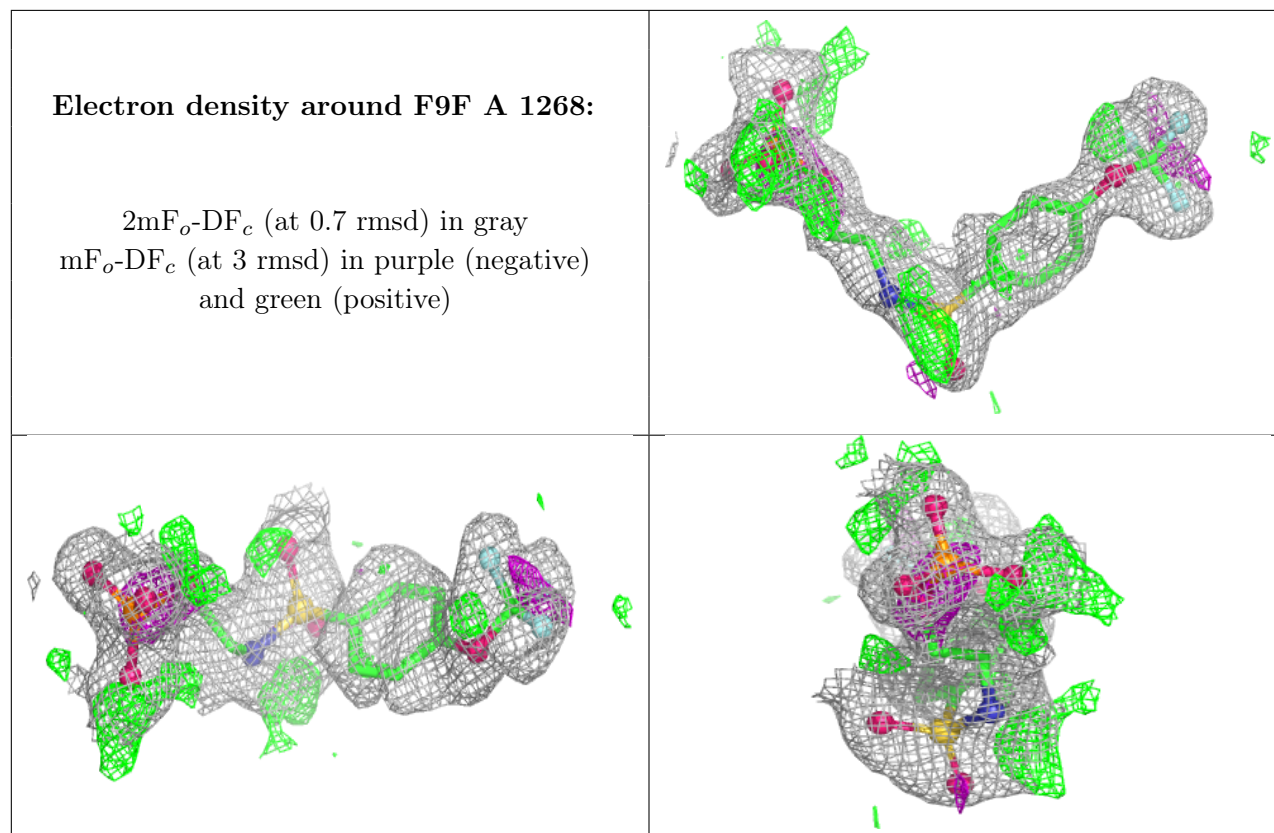
There are no oligosaccharides in this entry.

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.

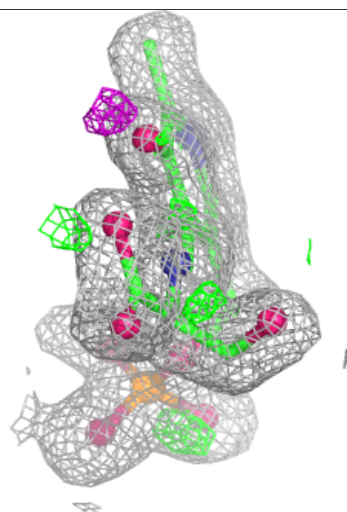
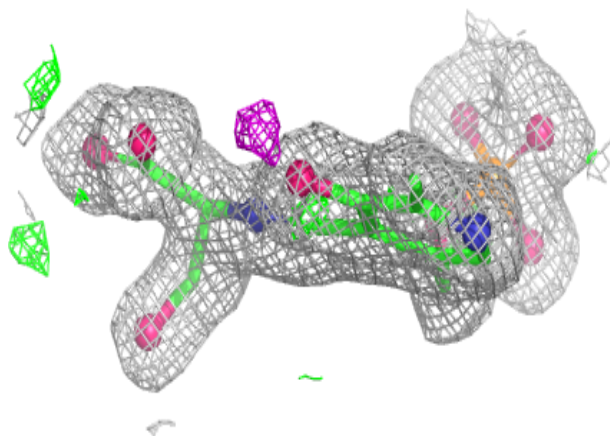
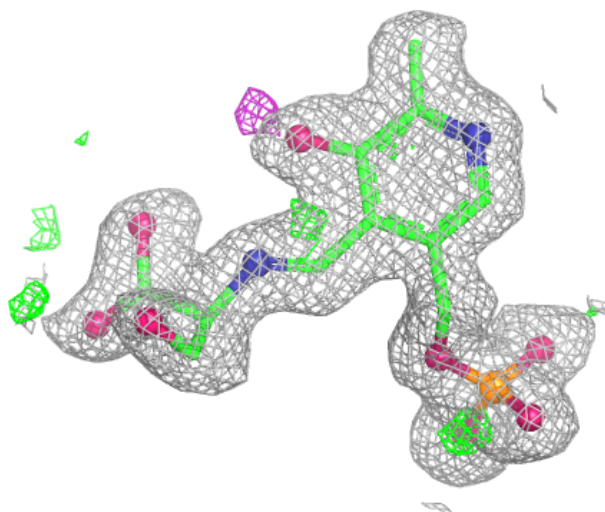
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	F9F	A	1268	22/22	0.85	0.14	19,31,34,35	0
4	PLS	B	1395	22/22	0.96	0.07	8,15,21,23	0
5	NA	B	1396	1/1	0.99	0.06	14,14,14,14	0

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 1395:

$2mF_o-DF_c$ (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.