



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:05 PM UTC

PDB ID : 2CLM / pdb_00002clm
Title : Tryptophan Synthase (external aldimine state) in complex with N-(4'- trifluoromethoxybenzoyl)-2-amino-1-ethylphosphate (F6F)
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 : 1.51 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

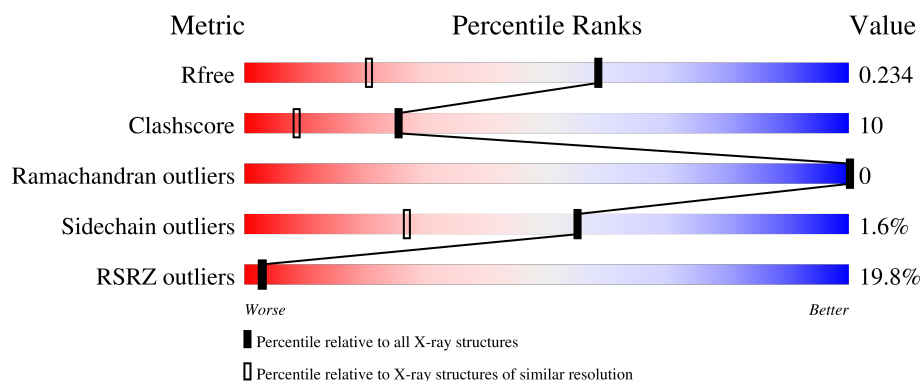
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	28% 67% 26% 6%
2	B	396	13% 84% 15% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5557 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	252	Total	C	N	O	S	0	0	1
			1902	1211	329	355	7			

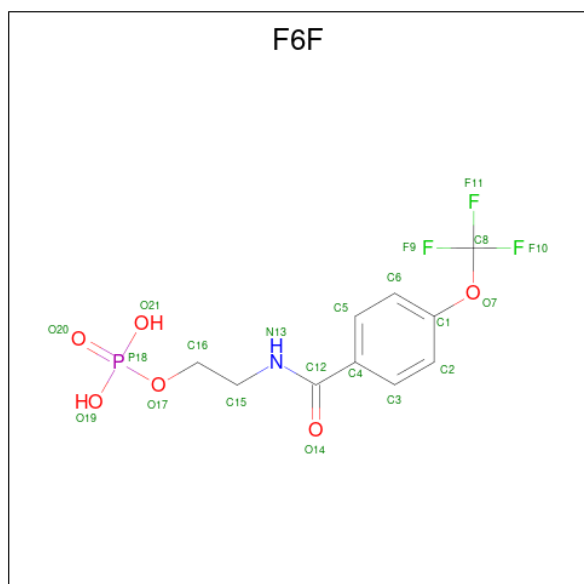
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	393	Total	C	N	O	S	0	0	1
			2968	1865	522	562	19			

There is a discrepancy between the modelled and reference sequences:

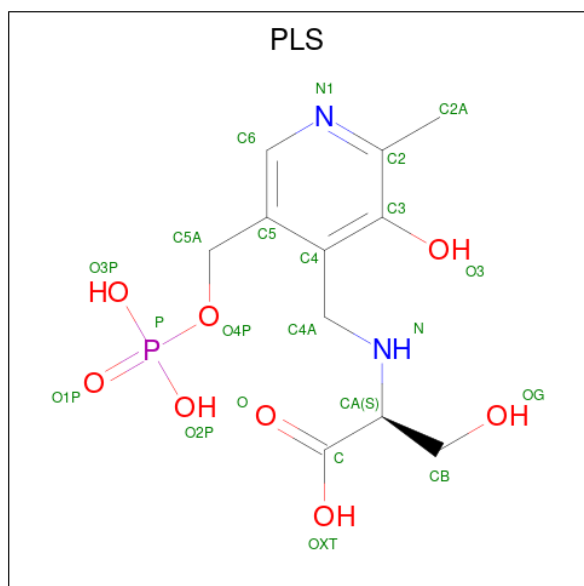
Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ARG	SER	conflict	UNP P0A2K1

- Molecule 3 is 2-{[4-(TRIFLUOROMETHOXY)BENZOYL]AMINO}ETHYL DIHYDROGEN PHOSPHATE (CCD ID: F6F) (formula: C₁₀H₁₁F₃NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	
			21	10	3	1	6	1	
								0	0

- Molecule 4 is [3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (CCD ID: PLS) (formula: C₁₁H₁₇N₂O₈P).



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

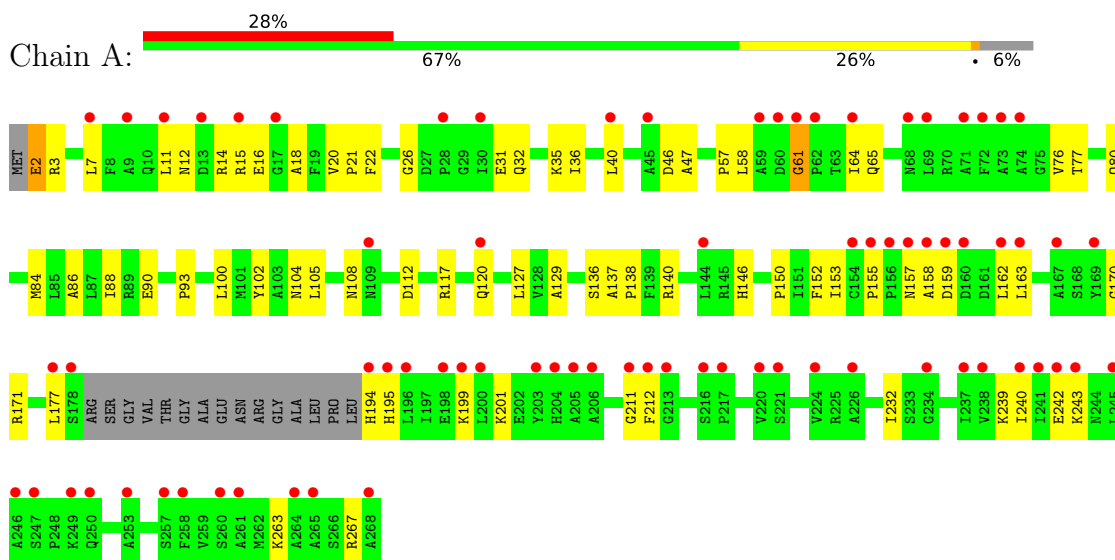
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	201	Total O		
			201 201	0	0
6	B	442	Total O		
			442 442	0	0

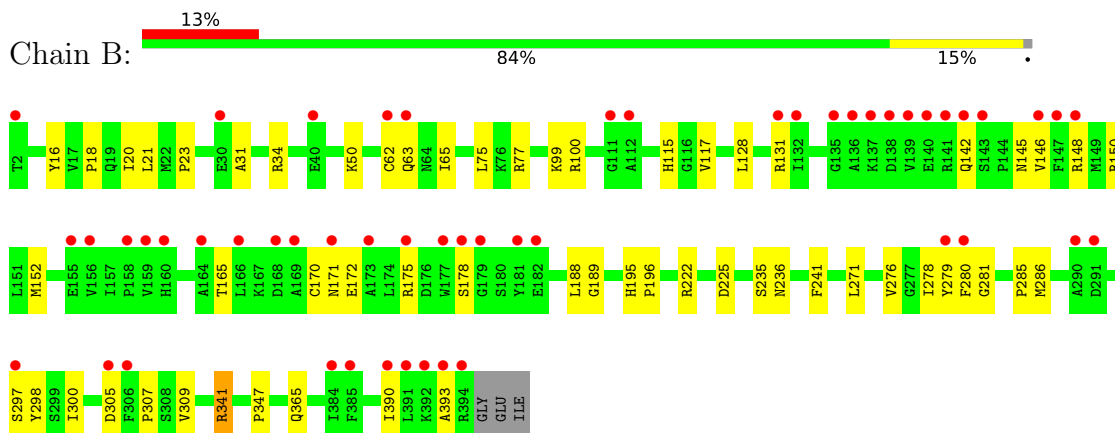
3 Residue-property plots [i](#)

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	182.51Å 59.54Å 67.71Å 90.00° 94.84° 90.00°	Depositor
Resolution (Å)	19.93 – 1.51 19.93 – 1.51	Depositor EDS
% Data completeness (in resolution range)	89.7 (19.93-1.51) 90.4 (19.93-1.51)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.239 0.214 , 0.234	Depositor DCC
R_{free} test set	5137 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 39.8	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	0.95	EDS
Total number of atoms	5557	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: F6F, NA, PLS

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	0.36	1/1940 (0.1%)	0.84	5/2636 (0.2%)
2	B	0.38	1/3026 (0.0%)	0.90	8/4090 (0.2%)
All	All	0.37	2/4966 (0.0%)	0.88	13/6726 (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)
2	B	393	ALA	C-N	-5.49	1.25	1.33
1	A	267	ARG	C-N	-5.35	1.25	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	SER	N-CA-C	7.49	122.18	112.89
2	B	365	GLN	CA-C-N	6.82	127.38	119.47
2	B	365	GLN	C-N-CA	6.82	127.38	119.47
2	B	77	ARG	N-CA-C	6.62	120.97	110.70
1	A	93	PRO	N-CA-C	5.66	120.93	113.86
2	B	195	HIS	N-CA-C	-5.53	102.61	109.64
1	A	129	ALA	N-CA-C	5.44	117.64	111.11
2	B	225	ASP	N-CA-C	-5.38	105.45	112.23
2	B	235	SER	N-CA-C	5.24	116.80	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	PHE	N-CA-C	5.20	117.03	111.36
1	A	61	GLY	CA-C-N	5.07	124.24	118.97
1	A	61	GLY	C-N-CA	5.07	124.24	118.97
2	B	305	ASP	N-CA-C	5.05	119.45	113.28

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	1902	0	1903	52	0
2	B	2968	0	2940	45	0
3	A	21	0	9	1	0
4	B	22	0	13	0	0
5	B	1	0	0	0	0
6	A	201	0	0	4	0
6	B	442	0	0	6	1
All	All	5557	0	4865	94	1

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 10.

All (94) 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:137:ALA:HB3	1:A:138:PRO:HD3	1.70	0.73
1:A:117:ARG:HH11	1:A:120:GLN:NE2	1.87	0.73
1:A:150:PRO:HD2	1:A:171:ARG:HB2	1.73	0.70
1:A:36:ILE:O	1:A:40:LEU:HD13	1.94	0.68
2:B:99:LYS:HD3	2:B:128:LEU:HD21	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ASN:HD22	2:B:148:ARG:HE	1.44	0.65
2:B:34:ARG:HG3	2:B:100:ARG:HE	1.60	0.65
1:A:140:ARG:HD3	1:A:152:PHE:HZ	1.61	0.64
1:A:159:ASP:O	1:A:163:LEU:HD13	1.99	0.63
2:B:172:GLU:HA	2:B:175:ARG:HD2	1.80	0.63
1:A:240:ILE:HA	1:A:243:LYS:HE3	1.82	0.62
2:B:63:GLN:HG2	6:B:2403:HOH:O	1.98	0.62
2:B:171:ASN:O	2:B:175:ARG:HG2	2.00	0.61
1:A:117:ARG:NH1	1:A:120:GLN:NE2	2.48	0.61
2:B:341:ARG:HG3	2:B:341:ARG:HH11	1.66	0.61
1:A:194:HIS:CD2	1:A:195:HIS:H	2.21	0.59
2:B:150:ARG:NH1	6:B:2244:HOH:O	2.33	0.58
1:A:155:PRO:HG2	1:A:158:ALA:HB2	1.87	0.56
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.89	0.55
1:A:211:GLY:O	1:A:212:PHE:HB2	2.06	0.55
2:B:62:CYS:SG	2:B:75:LEU:HG	2.47	0.55
2:B:172:GLU:HA	2:B:175:ARG:CG	2.37	0.54
1:A:32:GLN:O	1:A:36:ILE:HG13	2.08	0.54
1:A:100:LEU:C	1:A:100:LEU:HD13	2.33	0.53
1:A:140:ARG:HD3	1:A:152:PHE:CZ	2.44	0.53
2:B:99:LYS:CD	2:B:128:LEU:HD21	2.39	0.53
2:B:172:GLU:HA	2:B:175:ARG:CD	2.39	0.53
1:A:155:PRO:HA	1:A:177:LEU:HD12	1.90	0.52
2:B:297:SER:OG	2:B:307:PRO:HA	2.08	0.52
1:A:2:GLU:HG2	1:A:3:ARG:N	2.25	0.51
2:B:34:ARG:HG3	2:B:100:ARG:NE	2.26	0.51
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.45	0.51
2:B:145:ASN:ND2	2:B:148:ARG:HH21	2.08	0.51
1:A:22:PHE:C	1:A:22:PHE:CD1	2.89	0.50
1:A:170:GLY:O	1:A:171:ARG:HD2	2.11	0.50
2:B:222:ARG:NH2	6:B:2297:HOH:O	2.45	0.49
2:B:62:CYS:CB	2:B:65:ILE:HD11	2.43	0.48
1:A:46:ASP:OD2	1:A:263:LYS:HE2	2.13	0.48
1:A:117:ARG:O	1:A:120:GLN:HG2	2.13	0.48
2:B:62:CYS:HB3	2:B:65:ILE:HD11	1.96	0.48
1:A:12:ASN:O	1:A:15:ARG:HD2	2.14	0.47
2:B:341:ARG:HG3	2:B:341:ARG:NH1	2.28	0.47
1:A:158:ALA:CB	1:A:162:LEU:HD23	2.45	0.46
2:B:142:GLN:O	2:B:146:VAL:HG23	2.15	0.46
1:A:15:ARG:HD2	1:A:15:ARG:N	2.31	0.46
1:A:20:VAL:HG22	1:A:47:ALA:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:LEU:HD21	2:B:178:SER:HA	1.98	0.46
2:B:31:ALA:O	2:B:34:ARG:HG2	2.16	0.46
2:B:34:ARG:CG	2:B:100:ARG:HE	2.25	0.46
2:B:131:ARG:NH1	6:B:2218:HOH:O	2.49	0.46
2:B:16:TYR:O	2:B:281:GLY:HA2	2.17	0.45
2:B:285:PRO:C	2:B:286:MET:HG2	2.42	0.45
1:A:11:LEU:CD1	1:A:18:ALA:HB2	2.46	0.45
1:A:20:VAL:HB	1:A:232:ILE:HG12	1.99	0.45
1:A:158:ALA:HB1	1:A:162:LEU:HD23	1.99	0.45
1:A:16:GLU:HB3	6:A:2023:HOH:O	2.17	0.45
2:B:31:ALA:HA	2:B:34:ARG:HG2	1.99	0.44
2:B:150:ARG:HH11	2:B:150:ARG:HG2	1.82	0.44
1:A:61:GLY:O	1:A:65:GLN:HG3	2.18	0.43
2:B:34:ARG:CD	2:B:100:ARG:HE	2.30	0.43
1:A:77:THR:OG1	1:A:80:GLN:HG3	2.18	0.43
1:A:108:ASN:HA	6:A:2099:HOH:O	2.18	0.43
1:A:11:LEU:HD23	1:A:14:ARG:HH21	1.83	0.43
1:A:157:ASN:OD1	2:B:20:ILE:HD12	2.19	0.43
2:B:170:CYS:HB3	2:B:280:PHE:CE1	2.53	0.43
2:B:271:LEU:HD23	2:B:271:LEU:C	2.43	0.43
1:A:153:ILE:HG23	1:A:177:LEU:HG	1.99	0.43
1:A:157:ASN:ND2	2:B:23:PRO:HG2	2.33	0.43
2:B:172:GLU:CD	2:B:175:ARG:HD2	2.44	0.43
1:A:7:LEU:O	1:A:11:LEU:HG	2.18	0.43
1:A:239:LYS:HA	1:A:242:GLU:HG2	1.99	0.43
2:B:21:LEU:CD2	2:B:178:SER:HA	2.48	0.42
2:B:276:VAL:HA	2:B:285:PRO:HA	2.01	0.42
2:B:18:PRO:HB2	2:B:20:ILE:HG22	2.02	0.42
1:A:86:ALA:O	1:A:90:GLU:HG3	2.19	0.42
1:A:194:HIS:HD2	1:A:195:HIS:H	1.67	0.42
2:B:50:LYS:HG3	6:B:2122:HOH:O	2.18	0.42
2:B:117:VAL:HG13	2:B:152:MET:HE1	2.02	0.42
2:B:300:ILE:HD11	2:B:390:ILE:CD1	2.50	0.42
1:A:112:ASP:OD1	1:A:146:HIS:HE1	2.03	0.42
2:B:165:THR:CG2	6:B:2354:HOH:O	2.68	0.42
2:B:279:TYR:HB3	2:B:286:MET:SD	2.60	0.42
1:A:31:GLU:O	1:A:35:LYS:HG3	2.20	0.41
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.54	0.41
1:A:117:ARG:NH1	1:A:120:GLN:HE21	2.15	0.41
1:A:21:PRO:HD2	1:A:47:ALA:O	2.21	0.41
1:A:31:GLU:HG2	6:A:2035:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD12	1:A:58:LEU:C	2.46	0.41
1:A:64:ILE:CD1	3:A:1268:F6F:H151	2.51	0.41
1:A:127:LEU:C	1:A:127:LEU:HD23	2.45	0.41
1:A:84:MET:O	1:A:88:ILE:HG13	2.21	0.40
1:A:104:ASN:HB2	2:B:278:ILE:O	2.21	0.40
2:B:285:PRO:HG2	2:B:309:VAL:HG12	2.04	0.40
1:A:201:LYS:HA	6:A:2166:HOH:O	2.20	0.40

All (1) 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)
6:B:2125:HOH:O	6:B:2125:HOH:O[2_655]	1.90	0.30

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	248/268 (92%)	241 (97%)	7 (3%)	0	100	100
2	B	391/396 (99%)	381 (97%)	10 (3%)	0	100	100
All	All	639/664 (96%)	622 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	197/208 (95%)	194 (98%)	3 (2%)	57	29
2	B	306/310 (99%)	301 (98%)	5 (2%)	55	27
All	All	503/518 (97%)	495 (98%)	8 (2%)	55	27

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	105	LEU
1	A	199	LYS
2	B	188	LEU
2	B	196	PRO
2	B	236	ASN
2	B	341	ARG
2	B	347	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	80	GLN
1	A	120	GLN
1	A	147	ASN
1	A	194	HIS
1	A	195	HIS
1	A	244	ASN
1	A	250	GLN
2	B	26	ASN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	F6F	A	1268	-	21,21,21	2.17	7 (33%)	29,30,30	2.09	5 (17%)
4	PLS	B	1394	-	22,22,22	4.11	12 (54%)	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	F6F	A	1268	-	-	6/17/17/17	0/1/1/1
4	PLS	B	1394	-	-	4/17/17/17	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1394	PLS	C3-C4	9.63	1.54	1.40
4	B	1394	PLS	C3-C2	8.92	1.50	1.41
4	B	1394	PLS	O-C	8.15	1.46	1.22
4	B	1394	PLS	C4A-N	-4.57	1.33	1.46
4	B	1394	PLS	C5-C4	4.27	1.46	1.40
4	B	1394	PLS	C2-N1	4.15	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1268	F6F	C5-C4	4.11	1.45	1.39
4	B	1394	PLS	C6-C5	4.03	1.45	1.37
3	A	1268	F6F	C6-C5	3.90	1.45	1.38
3	A	1268	F6F	C3-C4	3.78	1.45	1.39
4	B	1394	PLS	P-O3P	-3.78	1.40	1.54
4	B	1394	PLS	CA-C	3.68	1.62	1.52
3	A	1268	F6F	C6-C1	3.58	1.45	1.38
3	A	1268	F6F	C3-C2	3.38	1.44	1.38
3	A	1268	F6F	C2-C1	3.20	1.44	1.38
4	B	1394	PLS	C6-N1	3.00	1.40	1.34
4	B	1394	PLS	P-O2P	-2.84	1.44	1.54
4	B	1394	PLS	P-O4P	-2.42	1.52	1.60
3	A	1268	F6F	O7-C8	2.12	1.42	1.31

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1268	F6F	C4-C12-N13	-9.60	97.18	117.12
4	B	1394	PLS	C4A-N-CA	7.68	128.24	113.84
4	B	1394	PLS	O3P-P-O4P	7.45	126.10	106.67
4	B	1394	PLS	O3-C3-C2	4.16	126.21	117.58
4	B	1394	PLS	O4P-C5A-C5	3.91	116.69	109.36
4	B	1394	PLS	C6-N1-C2	3.85	126.17	119.20
4	B	1394	PLS	OXT-C-O	-2.91	117.47	124.08
3	A	1268	F6F	O14-C12-N13	-2.85	117.04	122.59
4	B	1394	PLS	C5-C6-N1	-2.69	119.46	123.83
4	B	1394	PLS	OXT-C-CA	2.56	122.17	113.51
3	A	1268	F6F	O21-P18-O20	2.51	120.62	110.83
4	B	1394	PLS	C4A-C4-C5	-2.48	117.04	119.75
3	A	1268	F6F	P18-O17-C16	-2.47	111.49	118.21
4	B	1394	PLS	C3-C2-N1	-2.43	117.89	120.96
4	B	1394	PLS	C4A-C4-C3	2.28	123.01	119.98
4	B	1394	PLS	CB-CA-N	2.26	115.64	109.05
3	A	1268	F6F	O14-C12-C4	-2.01	116.92	120.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1268	F6F	O14-C12-N13-C15
3	A	1268	F6F	N13-C15-C16-O17
4	B	1394	PLS	C-CA-N-C4A

Continued on next page...

Continued from previous page...

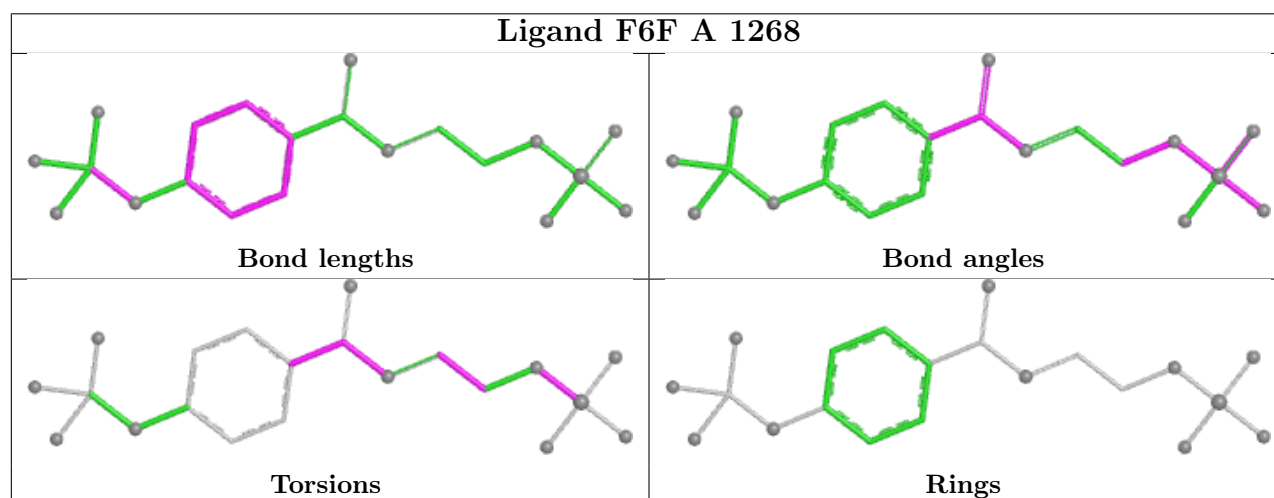
Mol	Chain	Res	Type	Atoms
4	B	1394	PLS	C3-C4-C4A-N
4	B	1394	PLS	C5-C4-C4A-N
3	A	1268	F6F	C4-C12-N13-C15
3	A	1268	F6F	N13-C12-C4-C3
3	A	1268	F6F	N13-C12-C4-C5
4	B	1394	PLS	CB-CA-N-C4A
3	A	1268	F6F	C16-O17-P18-O19

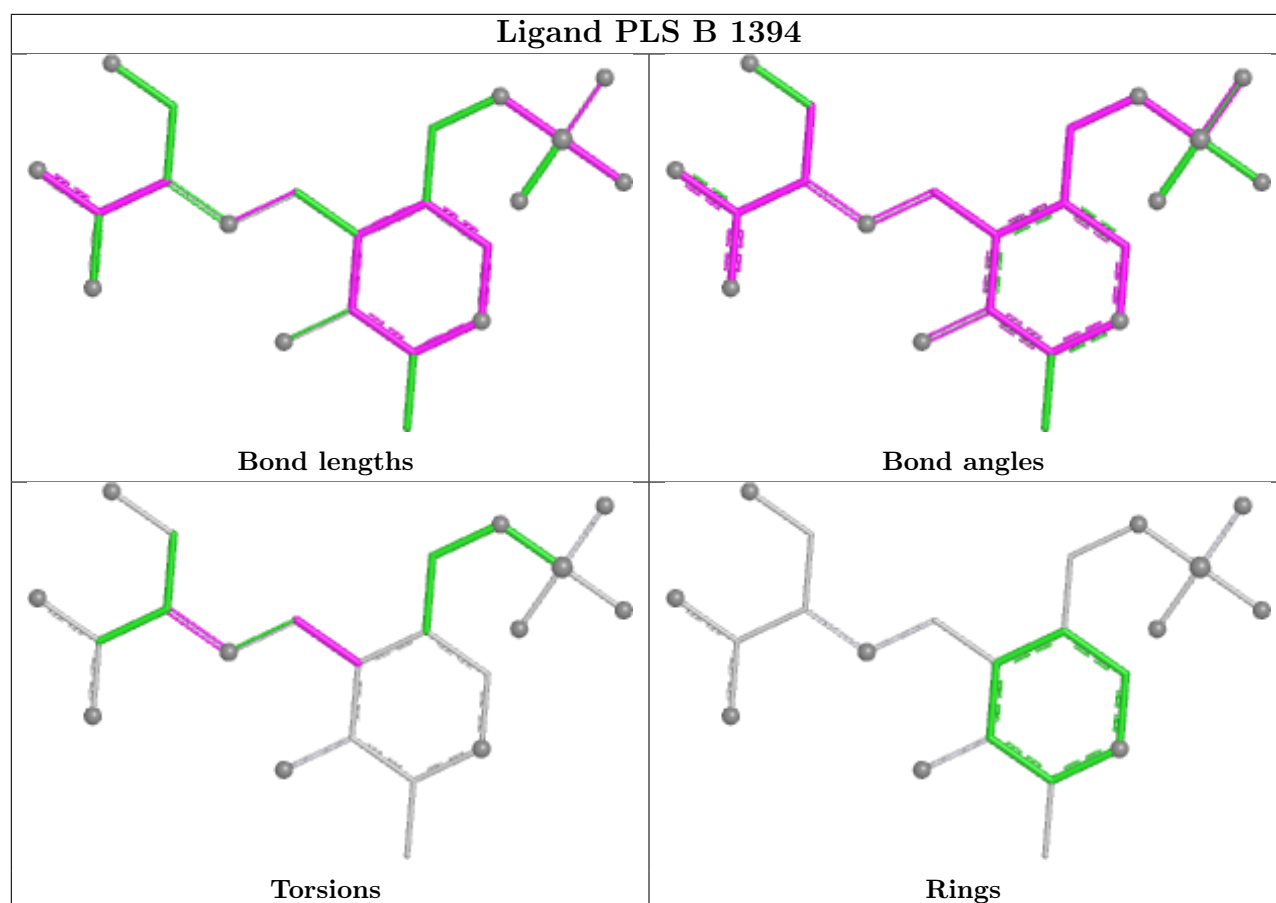
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1268	F6F	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	252/268 (94%)	1.46	76 (30%) 1 1	11, 27, 37, 44	0
2	B	393/396 (99%)	0.45	52 (13%) 7 9	9, 15, 32, 55	0
All	All	645/664 (97%)	0.84	128 (19%) 3 3	9, 20, 35, 55	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	391	LEU	6.1
1	A	177	LEU	5.1
2	B	62	CYS	4.9
1	A	194	HIS	4.8
1	A	195	HIS	4.8
1	A	245	LEU	4.7
1	A	158	ALA	4.7
2	B	393	ALA	4.6
2	B	390	ILE	4.4
1	A	69	LEU	4.2
2	B	181	TYR	3.9
2	B	384	ILE	3.9
2	B	146	VAL	3.9
1	A	268	ALA	3.8
1	A	220	VAL	3.7
2	B	135	GLY	3.7
1	A	224	VAL	3.7
2	B	140	GLU	3.6
2	B	164	ALA	3.6
2	B	394	ARG	3.6
1	A	213	GLY	3.6
1	A	72	PHE	3.6
1	A	226	ALA	3.5
2	B	63	GLN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	157	ASN	3.5
2	B	112	ALA	3.5
1	A	178	SER	3.5
1	A	247	SER	3.5
1	A	217	PRO	3.5
2	B	139	VAL	3.3
2	B	2	THR	3.2
2	B	280	PHE	3.2
2	B	385	PHE	3.2
1	A	258	PHE	3.1
1	A	264	ALA	3.1
1	A	242	GLU	3.0
2	B	40	GLU	3.0
2	B	182	GLU	3.0
1	A	265	ALA	3.0
2	B	136	ALA	3.0
1	A	198	GLU	2.9
1	A	163	LEU	2.9
2	B	178	SER	2.9
1	A	261	ALA	2.9
2	B	138	ASP	2.9
1	A	212	PHE	2.8
1	A	60	ASP	2.8
1	A	253	ALA	2.8
1	A	13	ASP	2.8
1	A	74	ALA	2.8
1	A	17	GLY	2.8
1	A	169	TYR	2.8
1	A	162	LEU	2.8
1	A	243	LYS	2.8
2	B	177	TRP	2.7
2	B	179	GLY	2.7
1	A	240	ILE	2.7
2	B	175	ARG	2.7
2	B	306	PHE	2.7
2	B	137	LYS	2.6
1	A	109	ASN	2.6
1	A	73	ALA	2.6
1	A	160	ASP	2.6
1	A	250	GLN	2.6
1	A	7	LEU	2.6
1	A	196	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	297	SER	2.6
2	B	132	ILE	2.6
2	B	173	ALA	2.6
2	B	166	LEU	2.6
1	A	155	PRO	2.6
1	A	9	ALA	2.5
1	A	167	ALA	2.5
1	A	61	GLY	2.5
2	B	111	GLY	2.5
1	A	15	ARG	2.5
2	B	131	ARG	2.5
2	B	142	GLN	2.5
1	A	11	LEU	2.5
1	A	200	LEU	2.5
1	A	28	PRO	2.5
2	B	159	VAL	2.5
1	A	203	TYR	2.4
2	B	171	ASN	2.4
1	A	260	SER	2.4
2	B	169	ALA	2.4
1	A	68	ASN	2.4
1	A	62	PRO	2.4
1	A	156	PRO	2.4
1	A	237	ILE	2.4
1	A	221	SER	2.4
1	A	59	ALA	2.4
2	B	305	ASP	2.3
1	A	238	VAL	2.3
2	B	155	GLU	2.3
1	A	211	GLY	2.3
1	A	234	GLY	2.3
2	B	160	HIS	2.3
2	B	147	PHE	2.3
1	A	64	ILE	2.3
2	B	143	SER	2.3
2	B	290	ALA	2.2
1	A	144	LEU	2.2
1	A	246	ALA	2.2
1	A	40	LEU	2.2
1	A	45	ALA	2.2
1	A	249	LYS	2.2
1	A	216	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	204	HIS	2.2
1	A	71	ALA	2.1
2	B	279	TYR	2.1
1	A	154	CYS	2.1
2	B	30	GLU	2.1
2	B	148	ARG	2.1
2	B	158	PRO	2.1
1	A	241	ILE	2.1
2	B	291	ASP	2.1
2	B	392	LYS	2.1
1	A	120	GLN	2.1
1	A	205	ALA	2.1
1	A	206	ALA	2.1
1	A	199	LYS	2.1
1	A	30	ILE	2.1
2	B	156	VAL	2.0
2	B	141	ARG	2.0
1	A	257	SER	2.0
1	A	159	ASP	2.0
2	B	168	ASP	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](#)

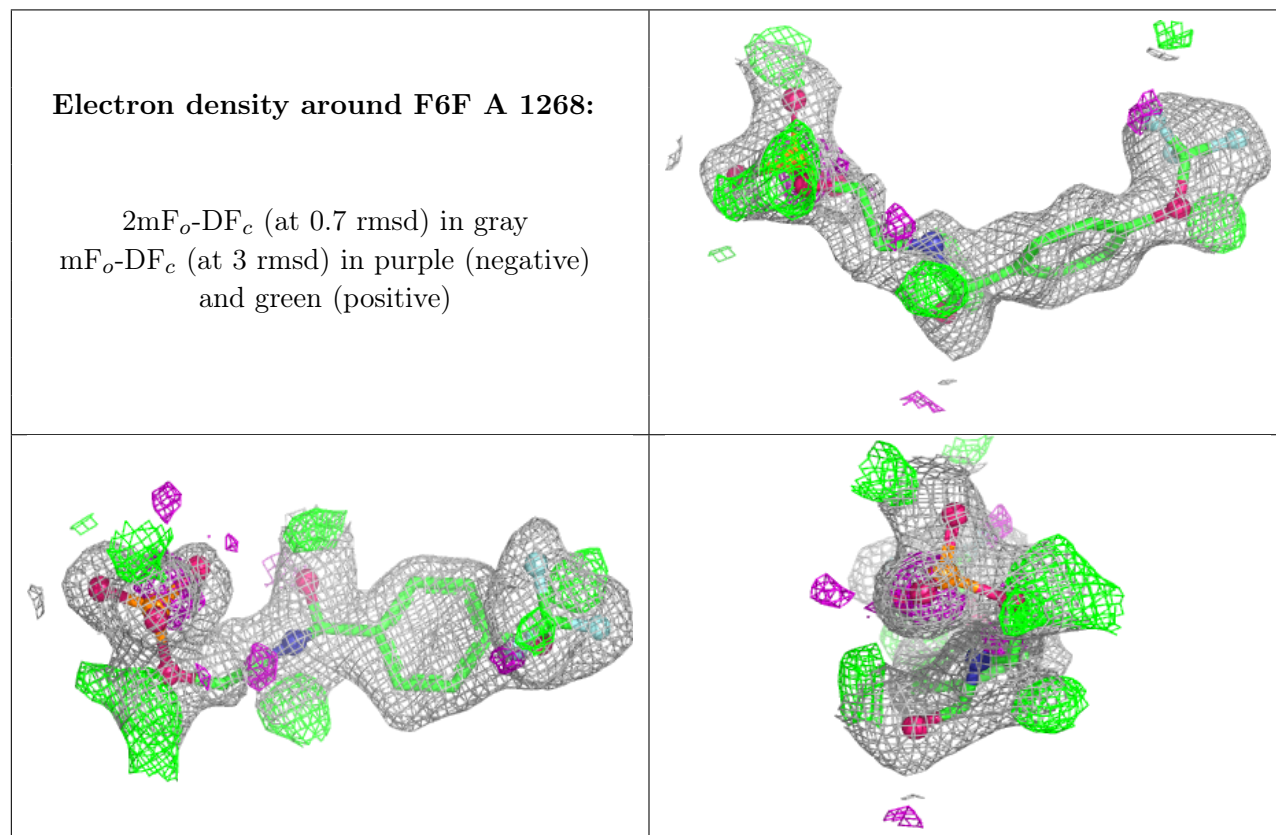
There are no oligosaccharides in this entry.

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.

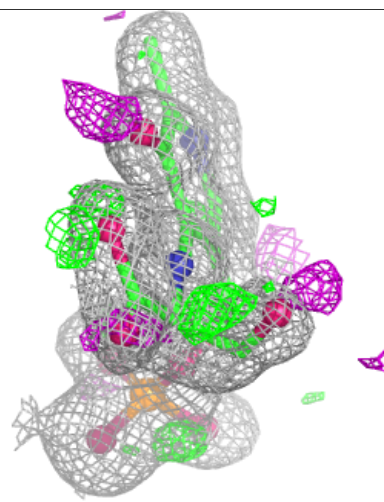
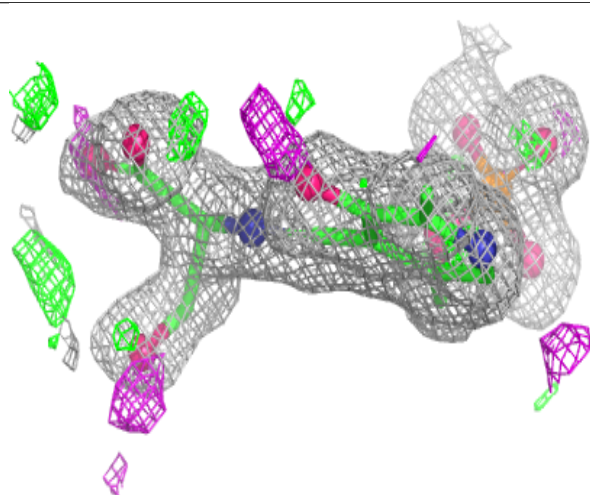
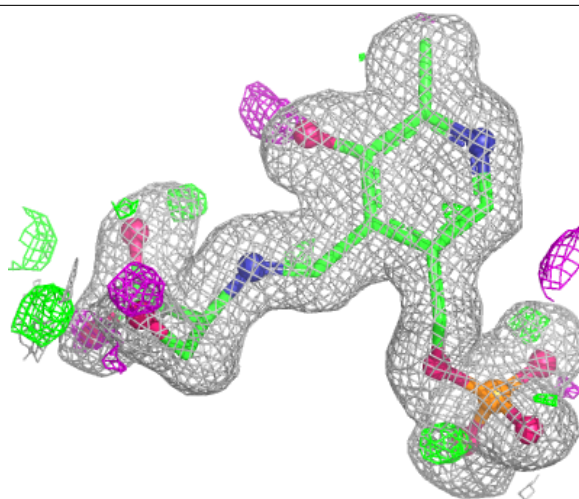
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	F6F	A	1268	21/21	0.80	0.13	29,31,35,37	0
4	PLS	B	1394	22/22	0.95	0.10	10,16,23,24	0
5	NA	B	1395	1/1	0.95	0.07	15,15,15,15	0

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 1394:

$2mF_o-DF_c$ (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.