



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:57 PM UTC

PDB ID : 2J9Y / pdb_00002j9y
Title : Tryptophan Synthase Q114N mutant in complex with Compound II
Authors : Blumenstein, L.; Domratcheva, T.; Niks, D.; Ngo, H.; Seidel, R.; Dunn, M.F.;
Schlichting, I.
Deposited on : 2006-11-16
Resolution : 1.80 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

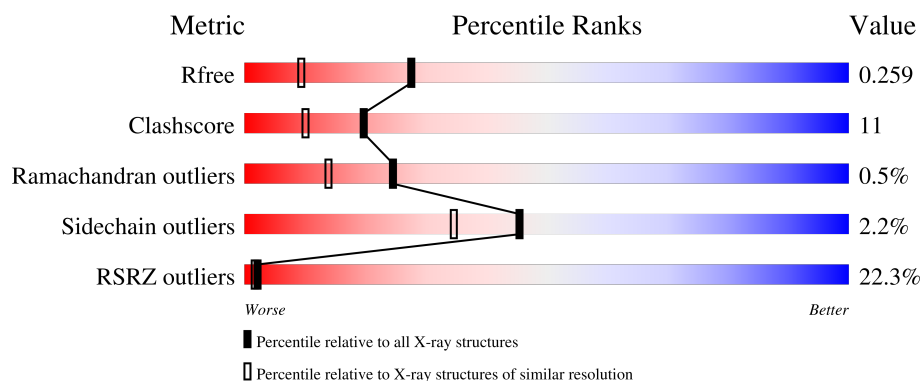
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	
2	B	397	

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
3	FOO	B	1396	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5448 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			

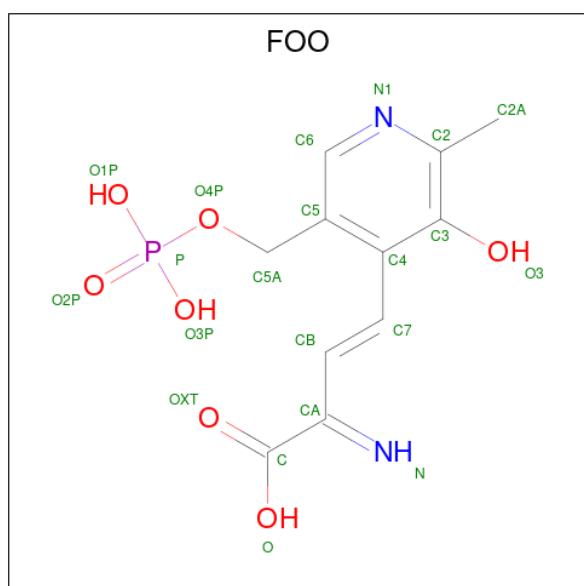
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	0	1
			2973	1867	523	564	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	ASN	GLN	engineered mutation	UNP P0A2K1

- Molecule 3 is (3E)-4-{3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}-2-IMINOBUT-3-ENOIC ACID (CCD ID: FOO) (formula: $C_{11}H_{13}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

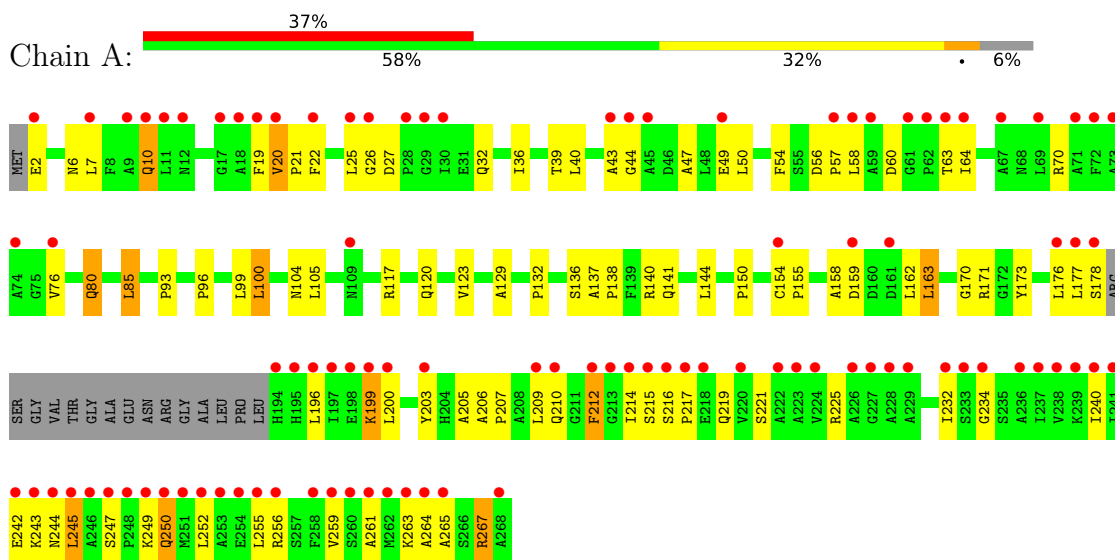
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total	O	0	0
			183	183		
5	B	368	Total	O	0	0
			368	368		

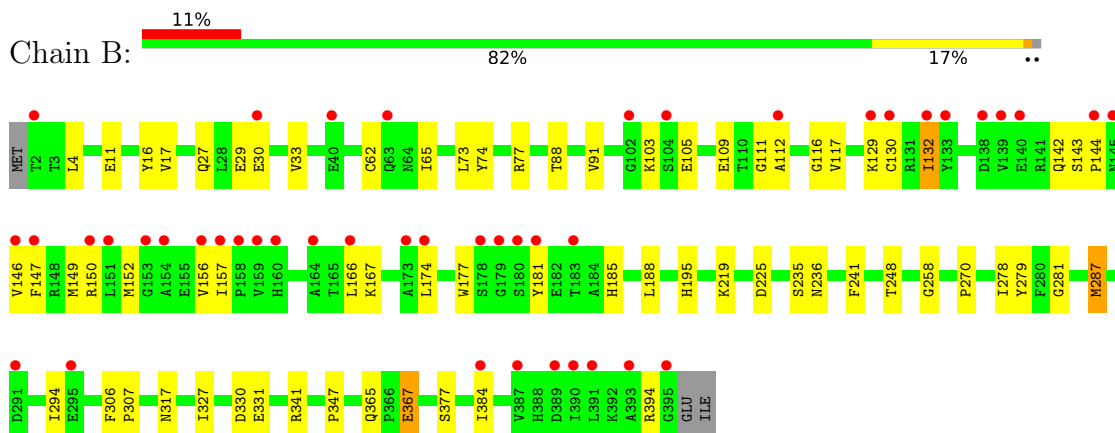
3 Residue-property plots

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

• Molecule 1: 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	182.74Å 60.70Å 67.41Å 90.00° 94.83° 90.00°	Depositor
Resolution (Å)	19.45 – 1.80 19.45 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.45-1.80) 98.8 (19.45-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.263 0.226 , 0.259	Depositor DCC
R_{free} test set	4003 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.845	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.1	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	5448	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FOO, 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	0.49	6/1940 (0.3%)	0.90	4/2636 (0.2%)
2	B	0.47	4/3031 (0.1%)	0.92	13/4097 (0.3%)
All	All	0.48	10/4971 (0.2%)	0.91	17/6733 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	ARG	C-N	-5.79	1.25	1.33
2	B	394	ARG	C-N	-5.74	1.25	1.33
2	B	317	ASN	CG-OD1	5.39	1.33	1.23
1	A	250	GLN	CD-OE1	5.28	1.33	1.23
2	B	142	GLN	CD-OE1	5.26	1.33	1.23
1	A	141	GLN	CD-OE1	5.25	1.33	1.23
1	A	80	GLN	CD-OE1	5.23	1.33	1.23
2	B	236	ASN	CG-OD1	5.17	1.33	1.23
1	A	10	GLN	CD-OE1	5.17	1.33	1.23
1	A	244	ASN	CG-OD1	5.06	1.33	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	77	ARG	N-CA-C	6.88	121.37	110.70
2	B	241	PHE	N-CA-C	6.80	118.49	111.14
1	A	136	SER	N-CA-C	6.79	120.83	112.54
1	A	20	VAL	N-CA-C	6.11	113.60	107.55
1	A	129	ALA	N-CA-C	6.04	118.64	111.33
2	B	287	MET	N-CA-C	-6.02	99.39	108.96
2	B	225	ASP	N-CA-C	-5.61	105.16	112.23
2	B	132	ILE	N-CA-C	5.55	115.94	108.17
2	B	235	SER	N-CA-C	5.54	117.13	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	HIS	N-CA-C	-5.49	102.21	109.84
2	B	377	SER	N-CA-C	5.42	117.94	111.71
2	B	365	GLN	CA-C-N	5.16	124.82	119.56
2	B	365	GLN	C-N-CA	5.16	124.82	119.56
2	B	248	THR	N-CA-C	5.04	118.21	111.75
1	A	93	PRO	N-CA-C	5.02	120.14	113.86
2	B	157	ILE	N-CA-C	5.02	112.97	107.60
2	B	130	CYS	N-CA-C	5.01	116.54	108.32

There are no chirality outliers.

There are no planarity outliers.

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	76	0
2	B	2973	0	2943	41	0
3	B	21	0	8	2	0
4	B	1	0	0	0	0
5	A	183	0	0	3	0
5	B	368	0	0	11	2
All	All	5448	0	4854	112	2

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 11.

All (112) 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:242:GLU:HA	1:A:245:LEU:HD13	1.47	0.94
2:B:167:LYS:HD3	2:B:307:PRO:HG3	1.50	0.93
1:A:155:PRO:HA	1:A:177:LEU:HD12	1.62	0.80
2:B:27:GLN:HB3	5:B:2065:HOH:O	1.86	0.76
1:A:159:ASP:O	1:A:163:LEU:HD22	1.87	0.74
1:A:210:GLN:HE21	1:A:214:ILE:HD11	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ALA:HA	1:A:267:ARG:NH1	2.05	0.72
2:B:117:VAL:HG13	2:B:152:MET:HE1	1.73	0.70
1:A:249:LYS:O	5:A:2174:HOH:O	2.12	0.68
1:A:263:LYS:O	1:A:263:LYS:HD3	1.92	0.68
2:B:74:TYR:HE2	5:B:2110:HOH:O	1.76	0.68
1:A:36:ILE:O	1:A:40:LEU:HD13	1.94	0.67
2:B:65:ILE:HD11	2:B:73:LEU:HD23	1.75	0.67
2:B:62:CYS:SG	2:B:65:ILE:HD11	2.35	0.66
1:A:6:ASN:O	1:A:10:GLN:HG3	1.96	0.66
1:A:196:LEU:O	1:A:196:LEU:HD23	1.96	0.65
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.79	0.65
1:A:20:VAL:HG22	1:A:47:ALA:HB3	1.81	0.63
1:A:22:PHE:HD2	1:A:49:GLU:HG3	1.64	0.63
1:A:176:LEU:HB3	1:A:210:GLN:HA	1.80	0.62
1:A:39:THR:HG23	1:A:256:ARG:HG2	1.82	0.62
1:A:140:ARG:O	1:A:144:LEU:HD13	2.00	0.62
1:A:216:SER:OG	1:A:219:GLN:HG3	1.99	0.61
1:A:199:LYS:HB3	1:A:203:TYR:CE2	2.35	0.61
1:A:210:GLN:HE21	1:A:214:ILE:CD1	2.15	0.59
1:A:264:ALA:HA	1:A:267:ARG:HH11	1.65	0.59
1:A:32:GLN:O	1:A:36:ILE:HG13	2.03	0.59
2:B:62:CYS:HB3	2:B:65:ILE:HG12	1.86	0.58
2:B:4:LEU:HD11	2:B:30:GLU:OE1	2.03	0.58
1:A:25:LEU:HD21	1:A:50:LEU:HD13	1.84	0.58
2:B:258:GLY:HA3	5:B:2265:HOH:O	2.03	0.58
1:A:19:PHE:HE2	1:A:259:VAL:HG13	1.70	0.56
1:A:25:LEU:HD11	1:A:85:LEU:HD11	1.88	0.56
1:A:2:GLU:N	5:A:2002:HOH:O	2.38	0.56
2:B:185:HIS:HA	5:B:2162:HOH:O	2.04	0.56
1:A:43:ALA:CB	1:A:259:VAL:HB	2.36	0.55
1:A:217:PRO:HB3	1:A:265:ALA:HB2	1.89	0.54
2:B:219:LYS:HE3	5:B:2109:HOH:O	2.06	0.54
2:B:270:PRO:HB3	2:B:287:MET:HG3	1.89	0.54
1:A:252:LEU:O	1:A:256:ARG:HG3	2.08	0.54
2:B:150:ARG:HE	2:B:156:VAL:HB	1.73	0.53
1:A:150:PRO:HD2	1:A:171:ARG:HB2	1.89	0.53
1:A:76:VAL:HA	1:A:80:GLN:HE21	1.73	0.53
2:B:103:LYS:HD3	5:B:2213:HOH:O	2.09	0.52
1:A:240:ILE:O	1:A:243:LYS:HG2	2.09	0.52
1:A:21:PRO:HD2	1:A:47:ALA:O	2.09	0.52
1:A:60:ASP:HB3	1:A:64:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:CYS:SG	1:A:196:LEU:HD21	2.50	0.51
2:B:109:GLU:CD	5:B:2165:HOH:O	2.54	0.50
1:A:170:GLY:O	1:A:171:ARG:HD2	2.11	0.50
1:A:43:ALA:HB1	1:A:259:VAL:HB	1.92	0.50
2:B:143:SER:O	2:B:147:PHE:HD1	1.94	0.50
1:A:173:TYR:HB2	1:A:209:LEU:HD13	1.94	0.50
1:A:100:LEU:C	1:A:100:LEU:HD13	2.37	0.49
1:A:178:SER:H	1:A:212:PHE:HB2	1.76	0.49
1:A:263:LYS:HD2	1:A:267:ARG:NH2	2.28	0.49
1:A:56:ASP:OD2	2:B:294:ILE:HB	2.13	0.49
2:B:167:LYS:HG3	2:B:279:TYR:OH	2.13	0.49
1:A:217:PRO:HG3	1:A:261:ALA:O	2.13	0.48
2:B:143:SER:OG	2:B:144:PRO:HD3	2.13	0.48
1:A:221:SER:HB3	1:A:225:ARG:HH12	1.78	0.48
1:A:206:ALA:O	1:A:207:PRO:C	2.56	0.48
2:B:341:ARG:HD2	5:B:2330:HOH:O	2.13	0.48
1:A:76:VAL:HA	1:A:80:GLN:NE2	2.29	0.48
1:A:58:LEU:C	1:A:58:LEU:HD12	2.39	0.47
1:A:132:PRO:HD3	2:B:17:VAL:O	2.14	0.47
1:A:20:VAL:HB	1:A:232:ILE:HG12	1.95	0.47
1:A:39:THR:CG2	1:A:256:ARG:HG2	2.44	0.47
1:A:58:LEU:HD22	2:B:174:LEU:HD12	1.97	0.47
1:A:54:PHE:O	1:A:57:PRO:HD3	2.15	0.46
1:A:199:LYS:N	1:A:199:LYS:HD2	2.29	0.46
1:A:216:SER:N	1:A:219:GLN:OE1	2.48	0.46
2:B:111:GLY:H	3:B:1396:FOO:C	2.28	0.46
2:B:367:GLU:HG2	5:B:2347:HOH:O	2.14	0.46
1:A:99:LEU:HD11	1:A:123:VAL:HG21	1.98	0.46
1:A:155:PRO:CA	1:A:177:LEU:HD12	2.41	0.46
1:A:117:ARG:NH1	1:A:120:GLN:OE1	2.47	0.46
1:A:7:LEU:HD22	1:A:96:PRO:HG2	1.98	0.45
1:A:255:LEU:O	1:A:259:VAL:HG23	2.16	0.45
1:A:19:PHE:CE2	1:A:259:VAL:HG13	2.50	0.45
2:B:146:VAL:HA	2:B:149:MET:HE3	1.98	0.45
1:A:22:PHE:C	1:A:22:PHE:CD1	2.95	0.44
2:B:112:ALA:HB3	3:B:1396:FOO:HB	1.98	0.44
1:A:263:LYS:HD3	1:A:263:LYS:C	2.43	0.44
2:B:177:TRP:O	2:B:181:TYR:HB3	2.16	0.44
1:A:247:SER:HB2	1:A:250:GLN:CG	2.48	0.44
2:B:306:PHE:CD1	2:B:307:PRO:HD2	2.52	0.44
2:B:11:GLU:O	2:B:11:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HB3	1:A:256:ARG:CZ	2.48	0.43
2:B:88:THR:O	2:B:91:VAL:HG22	2.17	0.43
1:A:247:SER:HB2	1:A:250:GLN:HG3	1.99	0.43
1:A:27:ASP:OD1	1:A:70:ARG:NE	2.49	0.43
1:A:215:SER:N	1:A:219:GLN:OE1	2.50	0.43
2:B:330:ASP:CG	5:B:2324:HOH:O	2.61	0.43
2:B:116:GLY:CA	2:B:132:ILE:HD13	2.49	0.43
1:A:58:LEU:HD22	2:B:174:LEU:CD1	2.49	0.42
2:B:327:ILE:HG23	2:B:331:GLU:HB2	2.00	0.42
2:B:166:LEU:HD23	2:B:306:PHE:HB2	2.01	0.42
1:A:104:ASN:HB2	2:B:278:ILE:O	2.20	0.42
1:A:158:ALA:HB1	1:A:162:LEU:HD23	2.02	0.42
2:B:219:LYS:HE3	5:B:2110:HOH:O	2.19	0.42
1:A:26:GLY:HA3	1:A:76:VAL:HG21	2.02	0.42
1:A:200:LEU:HB3	1:A:205:ALA:HB3	2.01	0.42
2:B:109:GLU:OE1	2:B:109:GLU:N	2.45	0.42
1:A:158:ALA:CB	1:A:162:LEU:HD23	2.49	0.42
1:A:178:SER:HB2	1:A:212:PHE:O	2.19	0.42
2:B:29:GLU:O	2:B:33:VAL:HG23	2.19	0.42
1:A:250:GLN:C	5:A:2174:HOH:O	2.63	0.41
2:B:105:GLU:HG2	2:B:129:LYS:HB3	2.02	0.41
1:A:177:LEU:O	1:A:178:SER:C	2.64	0.41
2:B:16:TYR:O	2:B:281:GLY:HA2	2.21	0.41
1:A:210:GLN:HG2	1:A:214:ILE:HD11	2.02	0.41

All (2) 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)
5:B:2151:HOH:O	5:B:2151:HOH:O[2_656]	2.00	0.20
5:B:2104:HOH:O	5:B:2104:HOH:O[2_655]	2.08	0.12

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	248/268 (92%)	235 (95%)	10 (4%)	3 (1%)	10	3
2	B	392/397 (99%)	384 (98%)	8 (2%)	0	100	100
All	All	640/665 (96%)	619 (97%)	18 (3%)	3 (0%)	24	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE
1	A	234	GLY
1	A	44	GLY

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	197/208 (95%)	190 (96%)	7 (4%)	31	18
2	B	307/311 (99%)	303 (99%)	4 (1%)	61	54
All	All	504/519 (97%)	493 (98%)	11 (2%)	45	34

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

Mol	Chain	Res	Type
1	A	63	THR
1	A	85	LEU
1	A	100	LEU
1	A	105	LEU
1	A	163	LEU
1	A	199	LYS
1	A	245	LEU
2	B	188	LEU
2	B	347	PRO
2	B	367	GLU

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Mol	Chain	Res	Type
2	B	384	ILE

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	66	ASN
1	A	68	ASN
1	A	80	GLN
1	A	109	ASN
1	A	141	GLN
1	A	165	GLN
1	A	195	HIS
1	A	210	GLN
2	B	44	GLN
2	B	246	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	FOO	B	1396	-	21,21,21	3.99	14 (66%)	25,30,30	3.06	12 (48%)

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	FOO	B	1396	-	-	2/10/15/15	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1396	FOO	C3-C2	10.94	1.52	1.41
3	B	1396	FOO	CA-C	-6.10	1.44	1.50
3	B	1396	FOO	OXT-C	5.53	1.36	1.22
3	B	1396	FOO	P-O4P	-5.22	1.43	1.60
3	B	1396	FOO	C6-C5	4.71	1.47	1.37
3	B	1396	FOO	C4-C3	3.94	1.47	1.41
3	B	1396	FOO	CA-N	-3.58	1.22	1.28
3	B	1396	FOO	P-O1P	-3.48	1.41	1.54
3	B	1396	FOO	C4-C7	-3.46	1.40	1.47
3	B	1396	FOO	P-O3P	-3.36	1.42	1.54
3	B	1396	FOO	CB-C7	2.93	1.40	1.33
3	B	1396	FOO	P-O2P	-2.69	1.42	1.50
3	B	1396	FOO	O-C	-2.38	1.24	1.30
3	B	1396	FOO	O3-C3	-2.16	1.31	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1396	FOO	O-C-CA	8.40	126.88	113.40
3	B	1396	FOO	O4P-C5A-C5	6.05	120.69	109.36
3	B	1396	FOO	O4P-P-O2P	5.36	120.94	106.44
3	B	1396	FOO	OXT-C-CA	-4.56	114.83	122.02
3	B	1396	FOO	C3-C4-C5	-4.02	115.05	118.28
3	B	1396	FOO	C5A-C5-C6	-3.84	113.09	119.36
3	B	1396	FOO	C7-CB-CA	2.62	128.60	125.38
3	B	1396	FOO	C4-C7-CB	2.56	134.29	128.50
3	B	1396	FOO	O-C-OXT	-2.49	117.97	123.90
3	B	1396	FOO	O1P-P-O4P	2.26	112.56	106.67
3	B	1396	FOO	O1P-P-O2P	-2.07	102.79	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1396	FOO	O3P-P-O1P	-2.06	100.06	107.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

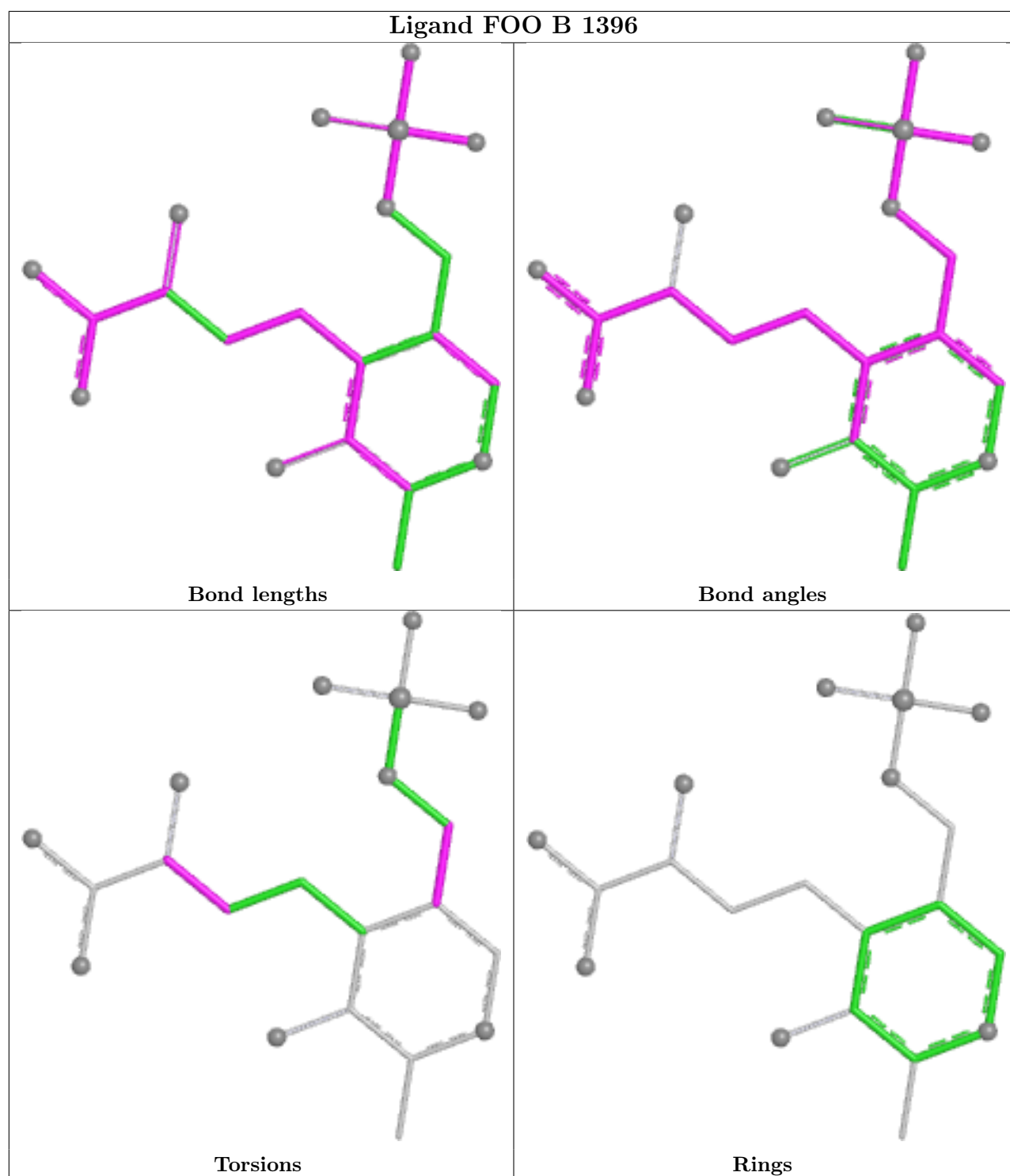
Mol	Chain	Res	Type	Atoms
3	B	1396	FOO	C4-C5-C5A-O4P
3	B	1396	FOO	C-CA-CB-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1396	FOO	2	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	252/268 (94%)	1.71	99 (39%) 1 0	18, 40, 50, 52	0
2	B	394/397 (99%)	0.35	45 (11%) 10 8	13, 20, 39, 49	0
All	All	646/665 (97%)	0.88	144 (22%) 2 2	13, 26, 48, 52	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ALA	5.9
1	A	212	PHE	5.9
1	A	245	LEU	5.6
2	B	164	ALA	4.9
1	A	214	ILE	4.8
1	A	255	LEU	4.8
1	A	264	ALA	4.7
1	A	258	PHE	4.6
1	A	196	LEU	4.5
1	A	194	HIS	4.4
1	A	62	PRO	4.4
2	B	156	VAL	4.3
1	A	229	ALA	4.2
1	A	234	GLY	4.1
1	A	237	ILE	4.1
1	A	222	ALA	4.1
1	A	236	ALA	4.1
2	B	154	ALA	4.1
1	A	30	ILE	4.1
1	A	265	ALA	4.1
1	A	17	GLY	4.1
2	B	147	PHE	4.0
2	B	157	ILE	4.0
1	A	259	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	216	SER	4.0
2	B	179	GLY	3.9
2	B	391	LEU	3.9
1	A	243	LYS	3.8
1	A	220	VAL	3.7
1	A	215	SER	3.6
1	A	195	HIS	3.6
1	A	252	LEU	3.6
1	A	244	ASN	3.6
1	A	251	MET	3.6
1	A	260	SER	3.6
1	A	176	LEU	3.6
1	A	18	ALA	3.6
1	A	67	ALA	3.5
1	A	74	ALA	3.5
2	B	63	GLN	3.4
2	B	395	GLY	3.4
1	A	73	ALA	3.4
1	A	232	ILE	3.4
1	A	261	ALA	3.4
2	B	129	LYS	3.3
2	B	144	PRO	3.3
1	A	238	VAL	3.3
2	B	158	PRO	3.3
1	A	247	SER	3.3
1	A	43	ALA	3.3
2	B	183	THR	3.3
1	A	242	GLU	3.2
1	A	218	GLU	3.2
1	A	217	PRO	3.2
1	A	26	GLY	3.1
2	B	102	GLY	3.1
1	A	240	ILE	3.1
1	A	210	GLN	3.1
2	B	178	SER	3.1
2	B	138	ASP	3.0
1	A	249	LYS	3.0
1	A	9	ALA	3.0
1	A	223	ALA	3.0
1	A	268	ALA	3.0
2	B	132	ILE	3.0
1	A	177	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	228	ALA	3.0
1	A	69	LEU	2.9
2	B	291	ASP	2.9
1	A	213	GLY	2.9
1	A	233	SER	2.9
2	B	146	VAL	2.9
1	A	198	GLU	2.9
2	B	151	LEU	2.9
2	B	390	ILE	2.9
1	A	72	PHE	2.8
2	B	166	LEU	2.8
1	A	154	CYS	2.8
2	B	139	VAL	2.8
1	A	253	ALA	2.8
1	A	209	LEU	2.8
2	B	174	LEU	2.8
2	B	181	TYR	2.7
1	A	109	ASN	2.7
1	A	71	ALA	2.7
2	B	173	ALA	2.7
1	A	11	LEU	2.7
1	A	197	ILE	2.7
1	A	256	ARG	2.7
1	A	20	VAL	2.7
2	B	130	CYS	2.6
1	A	19	PHE	2.6
1	A	25	LEU	2.6
1	A	224	VAL	2.6
1	A	250	GLN	2.6
1	A	58	LEU	2.6
1	A	2	GLU	2.6
2	B	104	SER	2.6
1	A	262	MET	2.5
2	B	389	ASP	2.5
2	B	2	THR	2.5
2	B	159	VAL	2.5
2	B	150	ARG	2.4
2	B	40	GLU	2.4
1	A	241	ILE	2.4
1	A	239	LYS	2.4
1	A	28	PRO	2.4
1	A	29	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	140	GLU	2.4
1	A	7	LEU	2.4
1	A	63	THR	2.4
1	A	61	GLY	2.4
1	A	200	LEU	2.3
1	A	254	GLU	2.3
2	B	112	ALA	2.3
1	A	203	TYR	2.3
1	A	248	PRO	2.3
1	A	45	ALA	2.3
1	A	159	ASP	2.3
1	A	44	GLY	2.2
1	A	227	GLY	2.2
2	B	180	SER	2.2
1	A	263	LYS	2.2
1	A	49	GLU	2.2
1	A	178	SER	2.2
2	B	153	GLY	2.2
2	B	133	TYR	2.2
1	A	10	GLN	2.1
1	A	57	PRO	2.1
1	A	59	ALA	2.1
1	A	161	ASP	2.1
2	B	295	GLU	2.1
1	A	22	PHE	2.1
1	A	12	ASN	2.1
1	A	226	ALA	2.1
2	B	145	ASN	2.0
2	B	387	VAL	2.0
2	B	393	ALA	2.0
2	B	30	GLU	2.0
1	A	199	LYS	2.0
1	A	64	ILE	2.0
2	B	160	HIS	2.0
2	B	384	ILE	2.0
1	A	76	VAL	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](#)

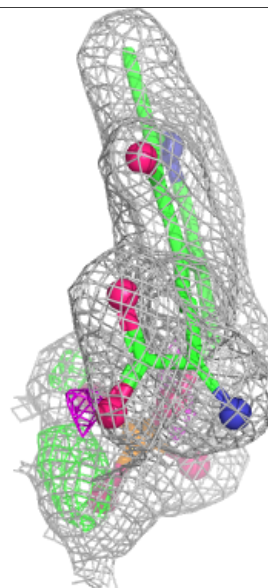
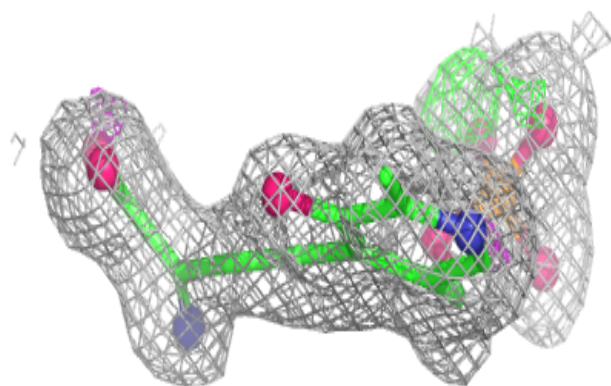
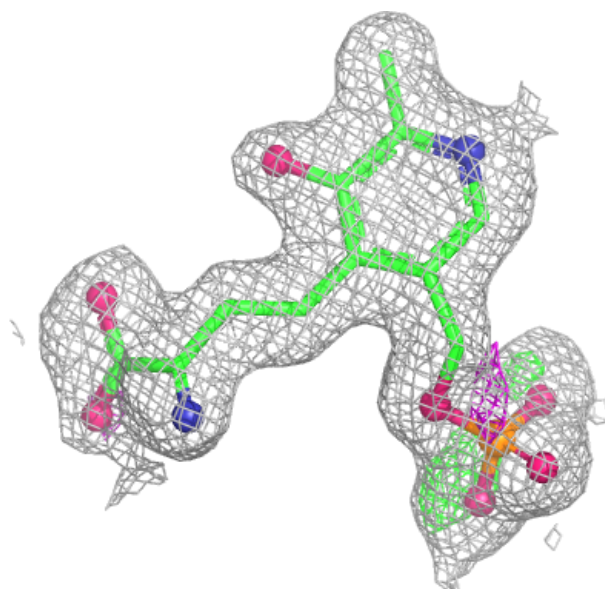
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FOO	B	1396	21/21	0.95	0.10	17,20,35,39	0
4	NA	B	1397	1/1	0.96	0.06	25,25,25,25	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 FOO B 1396:

$2mF_o-DF_c$ (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.