



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:27 PM UTC

PDB ID : 2DQ7 / pdb_00002dq7
Title : Crystal Structure of Fyn kinase domain complexed with staurosporine
Authors : Kinoshita, T.; Tada, T.
Deposited on : 2006-05-23
Resolution : 2.80 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

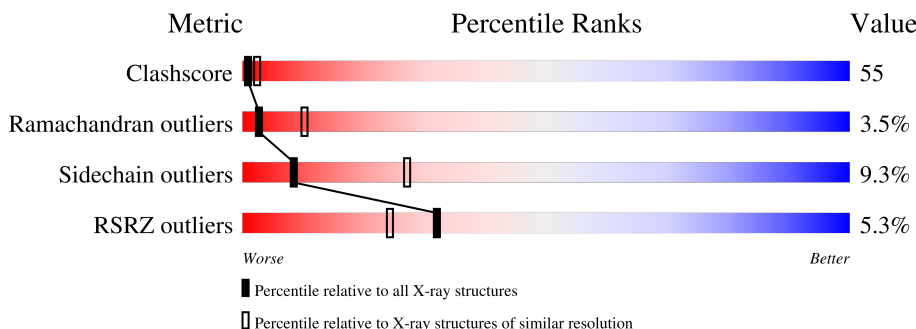
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	X	283	5% 33% 51% 9% 7%

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
1	PTR	X	160	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2286 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.

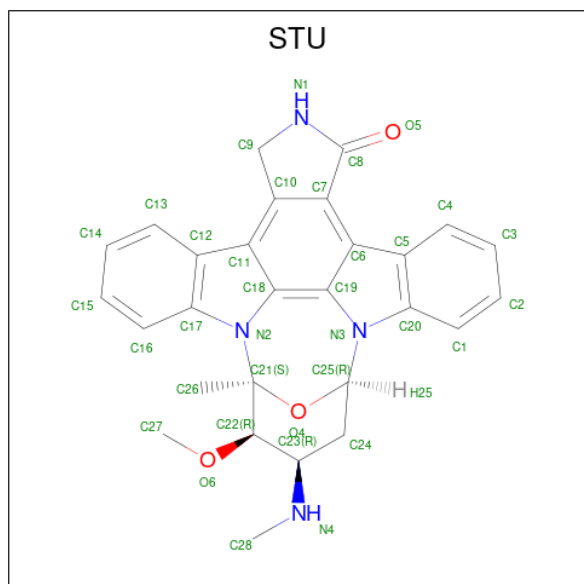
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Fyn.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	X	263	2121	1360	358	388	1	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	278	HIS	-	expression tag	UNP P06241
X	279	HIS	-	expression tag	UNP P06241
X	280	HIS	-	expression tag	UNP P06241
X	281	HIS	-	expression tag	UNP P06241
X	282	HIS	-	expression tag	UNP P06241
X	283	HIS	-	expression tag	UNP P06241

- Molecule 2 is STAUROSPORINE (CCD ID: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	X	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	130	Total	O	0	0
			130	130		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	52.96Å 52.96Å 210.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 99.9 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.05 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.281 0.268 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2286	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: PTR, STU

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	X	0.46	0/2152	1.03	10/2907 (0.3%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	236	HIS	N-CA-C	-8.90	101.24	112.90
1	X	233	ILE	N-CA-C	-7.51	101.37	111.44
1	X	254	GLU	N-CA-C	-7.13	103.20	110.97
1	X	207	TYR	CA-C-N	6.75	128.28	119.84
1	X	207	TYR	C-N-CA	6.75	128.28	119.84
1	X	74	SER	N-CA-C	6.67	121.13	113.19
1	X	237	GLU	N-CA-C	-5.88	105.37	112.54
1	X	86	ASN	N-CA-C	5.79	118.09	111.02
1	X	241	HIS	N-CA-C	-5.78	105.06	111.36
1	X	192	PHE	N-CA-C	-5.22	105.67	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	2121	0	2129	234	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	35	0	26	3	0
3	X	130	0	0	15	0
All	All	2286	0	2155	236	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 55.

All (236) 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:X:97:GLY:HA2	1:X:100:ARG:HD2	1.25	1.10
1:X:218:GLN:CG	1:X:223:TYR:HB2	1.83	1.07
1:X:100:ARG:O	1:X:202:LYS:HE3	1.60	0.99
1:X:218:GLN:HG2	1:X:223:TYR:HB2	1.01	0.99
1:X:218:GLN:HG2	1:X:223:TYR:CB	1.95	0.97
1:X:22:PHE:HA	1:X:45:THR:HG21	1.49	0.92
1:X:73:VAL:HB	1:X:79:TYR:HB2	1.54	0.90
1:X:87:LYS:HZ1	1:X:140:ASN:HA	1.37	0.90
1:X:96:ASP:HB2	1:X:98:GLU:OE2	1.71	0.89
1:X:71:ALA:HB3	1:X:81:VAL:HG21	1.58	0.86
1:X:102:LEU:HD22	1:X:106:ASN:HD22	1.43	0.82
1:X:170:ILE:HB	1:X:212:ASN:ND2	1.93	0.82
1:X:22:PHE:HD1	1:X:45:THR:CG2	1.91	0.82
1:X:97:GLY:HA2	1:X:100:ARG:CD	2.09	0.82
1:X:171:LYS:O	1:X:194:ILE:HD13	1.78	0.81
1:X:41:LEU:HD23	1:X:41:LEU:O	1.81	0.80
1:X:100:ARG:HD3	1:X:101:ALA:N	1.95	0.80
1:X:95:LYS:HE3	1:X:95:LYS:HA	1.66	0.77
1:X:182:ARG:HG3	1:X:182:ARG:O	1.84	0.77
1:X:160:PTR:HD2	1:X:161:THR:N	2.00	0.76
1:X:45:THR:HG22	1:X:46:MET:N	1.99	0.75
1:X:214:GLU:HA	3:X:937:HOH:O	1.86	0.75
1:X:71:ALA:N	1:X:81:VAL:HG23	2.02	0.74
1:X:97:GLY:CA	1:X:100:ARG:HD2	2.14	0.74
1:X:124:MET:HE2	1:X:124:MET:HA	1.68	0.74
1:X:98:GLU:CD	1:X:98:GLU:H	1.96	0.74
1:X:55:ALA:HB2	1:X:80:ILE:HD12	1.69	0.73
1:X:218:GLN:OE1	1:X:223:TYR:HB3	1.88	0.72
1:X:244:LYS:O	1:X:250:ARG:NH2	2.21	0.72
1:X:100:ARG:HD3	1:X:100:ARG:C	2.15	0.71
1:X:215:VAL:O	1:X:219:VAL:HG12	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:41:LEU:HD12	1:X:51:PHE:HB2	1.72	0.71
1:X:55:ALA:HB2	1:X:80:ILE:CD1	2.21	0.71
1:X:71:ALA:HB3	1:X:81:VAL:CG2	2.20	0.71
1:X:95:LYS:HE3	1:X:95:LYS:CA	2.20	0.70
1:X:151:LEU:HD13	1:X:168:PHE:HE2	1.56	0.70
1:X:21:GLN:N	3:X:935:HOH:O	2.25	0.69
1:X:241:HIS:CD2	1:X:251:PRO:HD3	2.28	0.68
2:X:902:STU:H16	2:X:902:STU:H261	1.76	0.68
1:X:107:LEU:HA	1:X:110:MET:HE3	1.76	0.68
1:X:55:ALA:O	1:X:59:LYS:HG3	1.94	0.68
1:X:96:ASP:HB2	1:X:98:GLU:CD	2.19	0.67
1:X:162:ALA:C	1:X:164:GLN:H	2.00	0.67
1:X:95:LYS:HA	1:X:95:LYS:CE	2.22	0.67
1:X:4:TRP:CH2	1:X:59:LYS:HB3	2.30	0.67
1:X:127:ILE:HB	1:X:155:ILE:HD11	1.76	0.66
1:X:224:ARG:HD2	1:X:243:TRP:HB3	1.76	0.66
1:X:96:ASP:O	1:X:100:ARG:HG3	1.96	0.66
1:X:65:LYS:NZ	1:X:113:GLN:HE21	1.94	0.66
1:X:134:ALA:HB1	2:X:902:STU:H281	1.77	0.65
1:X:96:ASP:CB	1:X:98:GLU:OE2	2.44	0.65
1:X:98:GLU:N	1:X:98:GLU:OE1	2.29	0.65
1:X:102:LEU:HD13	1:X:110:MET:HE1	1.78	0.65
1:X:87:LYS:NZ	1:X:140:ASN:HA	2.11	0.65
1:X:151:LEU:HD13	1:X:168:PHE:CE2	2.31	0.65
1:X:106:ASN:ND2	1:X:142:LEU:CD1	2.60	0.65
1:X:168:PHE:HB3	1:X:169:PRO:HD2	1.77	0.65
1:X:262:ASP:O	1:X:263:TYR:CD2	2.50	0.64
1:X:71:ALA:H	1:X:81:VAL:HG23	1.60	0.64
1:X:211:ASN:OD1	1:X:213:ARG:HB3	1.97	0.64
1:X:98:GLU:HG2	1:X:99:GLY:H	1.62	0.64
1:X:218:GLN:CG	1:X:223:TYR:CB	2.65	0.64
1:X:35:LYS:HE2	3:X:966:HOH:O	1.97	0.64
1:X:98:GLU:HG2	1:X:99:GLY:N	2.13	0.64
1:X:99:GLY:O	1:X:102:LEU:HB2	1.97	0.63
1:X:228:PRO:O	1:X:231:CYS:HB3	1.98	0.63
1:X:231:CYS:SG	1:X:235:LEU:HD11	2.38	0.63
1:X:12:GLN:N	1:X:12:GLN:OE1	2.32	0.63
1:X:22:PHE:CA	1:X:45:THR:HG21	2.26	0.63
2:X:902:STU:O5	2:X:902:STU:H4	1.99	0.63
1:X:211:ASN:OD1	1:X:214:GLU:HG3	1.98	0.62
1:X:153:ARG:HG3	1:X:160:PTR:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:87:LYS:HB2	1:X:138:VAL:HB	1.81	0.62
1:X:8:ARG:NH1	1:X:77:PRO:O	2.32	0.62
1:X:68:GLN:HG2	3:X:961:HOH:O	2.00	0.61
1:X:160:PTR:HD2	1:X:160:PTR:C	2.29	0.61
1:X:56:GLN:HA	1:X:56:GLN:OE1	2.01	0.61
1:X:60:LYS:HD2	1:X:60:LYS:O	2.01	0.61
1:X:100:ARG:CD	1:X:100:ARG:C	2.71	0.61
1:X:98:GLU:CG	1:X:99:GLY:H	2.14	0.60
1:X:87:LYS:HZ1	1:X:140:ASN:CA	2.13	0.60
1:X:102:LEU:HD13	1:X:110:MET:CE	2.31	0.60
1:X:22:PHE:CD1	1:X:45:THR:CG2	2.80	0.60
1:X:106:ASN:ND2	1:X:142:LEU:HD11	2.17	0.59
1:X:71:ALA:C	1:X:81:VAL:CG2	2.75	0.59
1:X:106:ASN:HD21	1:X:142:LEU:HD11	1.66	0.59
1:X:160:PTR:C	1:X:160:PTR:CD2	2.79	0.59
1:X:41:LEU:HD23	1:X:41:LEU:C	2.27	0.59
1:X:58:MET:HE1	1:X:82:THR:HG21	1.85	0.59
1:X:97:GLY:HA3	3:X:1022:HOH:O	2.03	0.59
1:X:96:ASP:O	1:X:100:ARG:CG	2.51	0.58
1:X:91:LEU:C	1:X:91:LEU:CD2	2.76	0.58
1:X:46:MET:HE3	1:X:51:PHE:HA	1.86	0.58
1:X:15:LYS:CE	1:X:27:MET:HE3	2.34	0.58
1:X:106:ASN:HD21	1:X:142:LEU:CD1	2.17	0.58
1:X:119:ALA:O	1:X:122:GLU:HB3	2.04	0.58
1:X:100:ARG:CD	1:X:101:ALA:N	2.65	0.57
1:X:67:VAL:HG21	1:X:147:ALA:HB2	1.85	0.57
1:X:182:ARG:O	1:X:182:ARG:CG	2.52	0.57
1:X:211:ASN:CG	1:X:214:GLU:HG3	2.29	0.57
1:X:95:LYS:HD2	1:X:202:LYS:O	2.04	0.57
1:X:50:SER:O	1:X:51:PHE:C	2.48	0.56
1:X:194:ILE:O	1:X:197:THR:HB	2.05	0.56
1:X:104:LEU:HD22	1:X:108:VAL:HG23	1.87	0.56
1:X:229:GLN:O	1:X:230:ASP:C	2.49	0.56
1:X:118:MET:HB3	1:X:253:PHE:CD2	2.40	0.55
1:X:163:ARG:HB3	3:X:949:HOH:O	2.05	0.55
1:X:224:ARG:HD2	1:X:243:TRP:CB	2.36	0.55
1:X:96:ASP:C	1:X:100:ARG:HB3	2.31	0.55
1:X:78:ILE:O	1:X:79:TYR:HD1	1.89	0.55
1:X:153:ARG:HG3	1:X:160:PTR:HD1	1.88	0.55
1:X:22:PHE:HD1	1:X:45:THR:HG22	1.72	0.55
1:X:102:LEU:HD22	1:X:106:ASN:ND2	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:172:TRP:HE1	1:X:198:GLU:CD	2.14	0.55
1:X:15:LYS:HE2	1:X:27:MET:HE3	1.89	0.55
1:X:41:LEU:CD1	1:X:51:PHE:HB2	2.38	0.55
1:X:219:VAL:HG13	1:X:220:GLU:N	2.22	0.55
1:X:63:HIS:CD2	1:X:120:TYR:HB2	2.42	0.54
1:X:75:GLU:HA	1:X:75:GLU:OE1	2.08	0.54
1:X:71:ALA:CA	1:X:81:VAL:HG23	2.37	0.54
1:X:96:ASP:O	1:X:100:ARG:CB	2.55	0.54
1:X:162:ALA:C	1:X:164:GLN:N	2.61	0.54
1:X:153:ARG:HG3	1:X:160:PTR:CE1	2.37	0.54
1:X:221:ARG:HG2	1:X:221:ARG:HH21	1.73	0.54
1:X:98:GLU:CG	1:X:99:GLY:N	2.70	0.54
1:X:211:ASN:ND2	1:X:214:GLU:OE2	2.41	0.54
1:X:102:LEU:CD1	1:X:110:MET:HE1	2.38	0.53
1:X:121:ILE:HG23	1:X:126:TYR:HB2	1.90	0.53
1:X:100:ARG:HD3	1:X:101:ALA:CA	2.38	0.53
1:X:8:ARG:HB2	1:X:8:ARG:NH2	2.24	0.53
1:X:102:LEU:CD2	1:X:106:ASN:HD22	2.20	0.53
1:X:257:GLN:O	1:X:261:GLU:HB2	2.10	0.52
1:X:8:ARG:HB2	1:X:8:ARG:HH21	1.73	0.52
1:X:1:LYS:HD2	1:X:1:LYS:N	2.24	0.52
1:X:95:LYS:O	1:X:96:ASP:OD2	2.28	0.52
1:X:159:GLU:OE1	1:X:182:ARG:HD3	2.09	0.52
1:X:245:LYS:HE3	3:X:911:HOH:O	2.09	0.52
1:X:204:ARG:HG2	1:X:205:VAL:N	2.24	0.51
1:X:177:ALA:O	1:X:181:GLY:HA2	2.10	0.51
1:X:62:LYS:HB3	3:X:914:HOH:O	2.11	0.51
1:X:195:LEU:C	1:X:195:LEU:HD23	2.35	0.51
1:X:42:LYS:O	1:X:45:THR:HB	2.11	0.51
1:X:14:ILE:HD11	1:X:27:MET:SD	2.51	0.51
1:X:200:VAL:HG12	1:X:201:THR:HG23	1.92	0.51
1:X:194:ILE:HG13	1:X:243:TRP:HE1	1.74	0.50
1:X:210:MET:HE2	1:X:215:VAL:HA	1.92	0.50
1:X:91:LEU:HD23	1:X:91:LEU:O	2.11	0.50
1:X:13:LEU:HD12	1:X:13:LEU:N	2.27	0.50
1:X:99:GLY:HA2	1:X:102:LEU:HG	1.92	0.49
1:X:131:LEU:O	1:X:132:ARG:HB3	2.13	0.49
1:X:262:ASP:O	1:X:263:TYR:HD2	1.95	0.49
1:X:207:TYR:HB3	1:X:210:MET:HG3	1.95	0.49
1:X:71:ALA:C	1:X:81:VAL:HG23	2.38	0.48
1:X:12:GLN:HE22	1:X:32:GLY:H	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:100:ARG:HH21	1:X:101:ALA:HB2	1.77	0.48
1:X:120:TYR:HD1	1:X:123:ARG:HH11	1.62	0.48
1:X:237:GLU:OE1	1:X:240:ILE:HD11	2.13	0.48
1:X:87:LYS:HZ1	1:X:140:ASN:CG	2.22	0.47
1:X:65:LYS:NZ	1:X:113:GLN:NE2	2.62	0.47
1:X:124:MET:HE2	1:X:124:MET:CA	2.41	0.47
1:X:91:LEU:C	1:X:91:LEU:HD23	2.39	0.47
1:X:8:ARG:HH21	1:X:8:ARG:CB	2.28	0.47
1:X:15:LYS:NZ	1:X:27:MET:HE3	2.30	0.47
1:X:71:ALA:C	1:X:81:VAL:HG22	2.40	0.47
1:X:122:GLU:HG3	1:X:185:ILE:HG12	1.97	0.47
1:X:127:ILE:CD1	1:X:183:PHE:HB3	2.46	0.46
1:X:107:LEU:HD23	1:X:110:MET:CE	2.45	0.46
1:X:245:LYS:HG2	3:X:911:HOH:O	2.15	0.46
1:X:71:ALA:O	1:X:81:VAL:CG2	2.63	0.46
1:X:210:MET:CE	1:X:215:VAL:HA	2.46	0.46
1:X:96:ASP:O	1:X:100:ARG:HB3	2.15	0.46
1:X:235:LEU:HD12	1:X:235:LEU:C	2.41	0.46
1:X:96:ASP:HB2	1:X:98:GLU:OE1	2.15	0.46
1:X:156:GLU:HA	1:X:156:GLU:OE1	2.16	0.46
1:X:253:PHE:HA	1:X:256:LEU:HB2	1.98	0.46
1:X:46:MET:CG	1:X:47:SER:N	2.80	0.45
1:X:98:GLU:CD	1:X:98:GLU:N	2.64	0.45
1:X:210:MET:HG3	1:X:215:VAL:HG22	1.98	0.45
1:X:195:LEU:HD23	1:X:195:LEU:O	2.15	0.45
1:X:21:GLN:NE2	3:X:1017:HOH:O	2.49	0.45
1:X:113:GLN:HE22	1:X:143:ILE:HA	1.81	0.45
1:X:255:TYR:CD1	1:X:255:TYR:C	2.94	0.45
1:X:163:ARG:NH2	1:X:166:ALA:HB2	2.32	0.45
1:X:123:ARG:NE	3:X:941:HOH:O	2.49	0.45
1:X:218:GLN:OE1	1:X:223:TYR:CB	2.60	0.45
1:X:213:ARG:HG2	1:X:213:ARG:HH21	1.81	0.45
1:X:54:GLU:HG3	1:X:149:PHE:C	2.42	0.45
1:X:218:GLN:CD	1:X:223:TYR:CB	2.90	0.44
1:X:39:LYS:NZ	1:X:54:GLU:OE1	2.47	0.44
1:X:229:GLN:O	1:X:231:CYS:N	2.51	0.44
1:X:190:TRP:HE1	1:X:194:ILE:HD11	1.81	0.44
1:X:223:TYR:N	1:X:223:TYR:CD2	2.83	0.44
1:X:11:LEU:C	1:X:12:GLN:OE1	2.61	0.44
1:X:176:GLU:OE2	1:X:250:ARG:NH1	2.51	0.44
1:X:202:LYS:NZ	3:X:1010:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2:ASP:HB3	1:X:5:GLU:HB2	2.00	0.44
1:X:160:PTR:O2P	1:X:162:ALA:HA	2.17	0.43
1:X:6:ILE:HA	1:X:7:PRO:HD3	1.70	0.43
1:X:157:ASP:O	1:X:158:ASN:HB2	2.19	0.43
1:X:190:TRP:HE1	1:X:194:ILE:CD1	2.31	0.43
1:X:21:GLN:CD	3:X:1017:HOH:O	2.61	0.43
1:X:58:MET:HE1	1:X:82:THR:CG2	2.48	0.43
1:X:127:ILE:HD11	1:X:183:PHE:HB3	2.01	0.43
1:X:221:ARG:HG2	1:X:221:ARG:NH2	2.34	0.43
1:X:12:GLN:O	1:X:14:ILE:HG23	2.19	0.42
1:X:46:MET:CG	1:X:50:SER:HB2	2.49	0.42
1:X:104:LEU:HD22	1:X:108:VAL:CG2	2.48	0.42
1:X:162:ALA:O	1:X:164:GLN:N	2.52	0.42
1:X:231:CYS:SG	1:X:235:LEU:CD1	3.06	0.42
1:X:106:ASN:O	1:X:109:ASP:HB3	2.20	0.42
1:X:194:ILE:HG13	1:X:243:TRP:NE1	2.35	0.42
1:X:58:MET:HE2	1:X:69:LEU:HB2	2.02	0.42
1:X:211:ASN:O	1:X:214:GLU:N	2.52	0.42
1:X:90:LEU:HB3	1:X:133:SER:O	2.20	0.42
1:X:160:PTR:CD2	1:X:161:THR:N	2.78	0.42
1:X:126:TYR:CE1	1:X:154:LEU:HD13	2.55	0.41
1:X:127:ILE:O	1:X:152:ALA:HA	2.20	0.41
1:X:195:LEU:HA	1:X:198:GLU:OE1	2.20	0.41
1:X:220:GLU:C	1:X:222:GLY:H	2.27	0.41
1:X:41:LEU:HB2	1:X:51:PHE:CD1	2.56	0.41
1:X:13:LEU:N	1:X:13:LEU:CD1	2.83	0.41
1:X:71:ALA:O	1:X:81:VAL:HG22	2.20	0.41
1:X:1:LYS:N	1:X:1:LYS:CD	2.83	0.41
1:X:68:GLN:HA	3:X:945:HOH:O	2.20	0.41
1:X:104:LEU:HB3	1:X:105:PRO:CD	2.50	0.41
1:X:50:SER:HA	1:X:53:GLU:HG3	2.01	0.41
1:X:87:LYS:HB2	1:X:138:VAL:O	2.20	0.41
1:X:149:PHE:HA	3:X:948:HOH:O	2.20	0.41
1:X:170:ILE:HB	1:X:212:ASN:HD22	1.79	0.41
1:X:71:ALA:CB	1:X:81:VAL:CG2	2.95	0.41
1:X:190:TRP:CD1	1:X:190:TRP:C	2.99	0.41
1:X:78:ILE:HG22	1:X:79:TYR:N	2.35	0.40
1:X:90:LEU:HD22	1:X:136:ILE:HG21	2.01	0.40
1:X:30:TRP:NE1	1:X:31:ASN:ND2	2.70	0.40
1:X:235:LEU:C	1:X:235:LEU:CD1	2.95	0.40
1:X:71:ALA:CA	1:X:81:VAL:CG2	3.00	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	X	260/283 (92%)	227 (87%)	24 (9%)	9 (4%)	3	10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	156	GLU
1	X	158	ASN
1	X	208	PRO
1	X	230	ASP
1	X	170	ILE
1	X	169	PRO
1	X	212	ASN
1	X	104	LEU
1	X	43	PRO

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	X	226/244 (93%)	205 (91%)	21 (9%)	8	27

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	3	VAL
1	X	34	THR
1	X	41	LEU
1	X	49	GLU
1	X	56	GLN
1	X	60	LYS
1	X	68	GLN
1	X	91	LEU
1	X	98	GLU
1	X	100	ARG
1	X	104	LEU
1	X	106	ASN
1	X	182	ARG
1	X	200	VAL
1	X	208	PRO
1	X	210	MET
1	X	218	GLN
1	X	235	LEU
1	X	248	GLU
1	X	256	LEU
1	X	263	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	21	GLN
1	X	31	ASN
1	X	106	ASN
1	X	113	GLN
1	X	257	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PTR	X	160	1	15,16,17	0.94	1 (6%)	17,22,24	1.60	4 (23%)

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
1	PTR	X	160	1	-	2/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	160	PTR	P-OH	-2.37	1.55	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	160	PTR	OH-P-O1P	-4.23	95.37	109.48
1	X	160	PTR	O3P-P-O2P	2.75	118.12	107.80
1	X	160	PTR	O2P-P-OH	-2.27	98.59	105.32
1	X	160	PTR	O3P-P-OH	-2.17	98.89	105.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	X	160	PTR	CA-CB-CG-CD2
1	X	160	PTR	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	X	160	PTR	8	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	STU	X	902	-	39,42,42	1.96	11 (28%)	50,68,68	3.05	18 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STU	X	902	-	-	1/4/42/42	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	902	STU	C9-N1	4.08	1.49	1.45
2	X	902	STU	C17-N2	-3.66	1.36	1.40
2	X	902	STU	C18-N2	-3.60	1.36	1.40
2	X	902	STU	C8-N1	3.10	1.37	1.35
2	X	902	STU	C14-C13	3.00	1.44	1.38
2	X	902	STU	C26-C21	3.00	1.54	1.51
2	X	902	STU	C2-C1	2.81	1.43	1.38
2	X	902	STU	C20-N3	-2.77	1.36	1.40
2	X	902	STU	C7-C8	-2.64	1.40	1.49
2	X	902	STU	C3-C4	2.61	1.43	1.38
2	X	902	STU	C19-N3	-2.28	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	902	STU	C9-C10-C7	-9.86	106.26	109.88
2	X	902	STU	C9-C10-C11	8.89	135.48	128.73
2	X	902	STU	C12-C17-N2	7.32	113.76	108.94
2	X	902	STU	C10-C7-C8	6.49	113.52	108.09
2	X	902	STU	C11-C10-C7	-4.54	118.26	121.25
2	X	902	STU	C18-C11-C10	4.47	125.04	119.77
2	X	902	STU	C11-C12-C17	-3.99	102.47	106.49
2	X	902	STU	C6-C5-C20	-3.64	102.82	106.49
2	X	902	STU	C6-C7-C10	-3.54	118.29	120.76
2	X	902	STU	C13-C12-C17	3.46	123.24	119.24
2	X	902	STU	C18-C19-N3	3.23	132.17	129.42
2	X	902	STU	C16-C17-C12	-3.17	117.88	121.59
2	X	902	STU	C7-C6-C19	2.89	122.89	118.04
2	X	902	STU	C24-C23-C22	-2.65	104.45	109.53
2	X	902	STU	C4-C5-C20	2.63	122.28	119.24
2	X	902	STU	C12-C11-C10	-2.61	127.59	132.33
2	X	902	STU	C19-C18-N2	2.43	133.44	131.38
2	X	902	STU	C11-C18-C19	-2.07	116.30	121.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

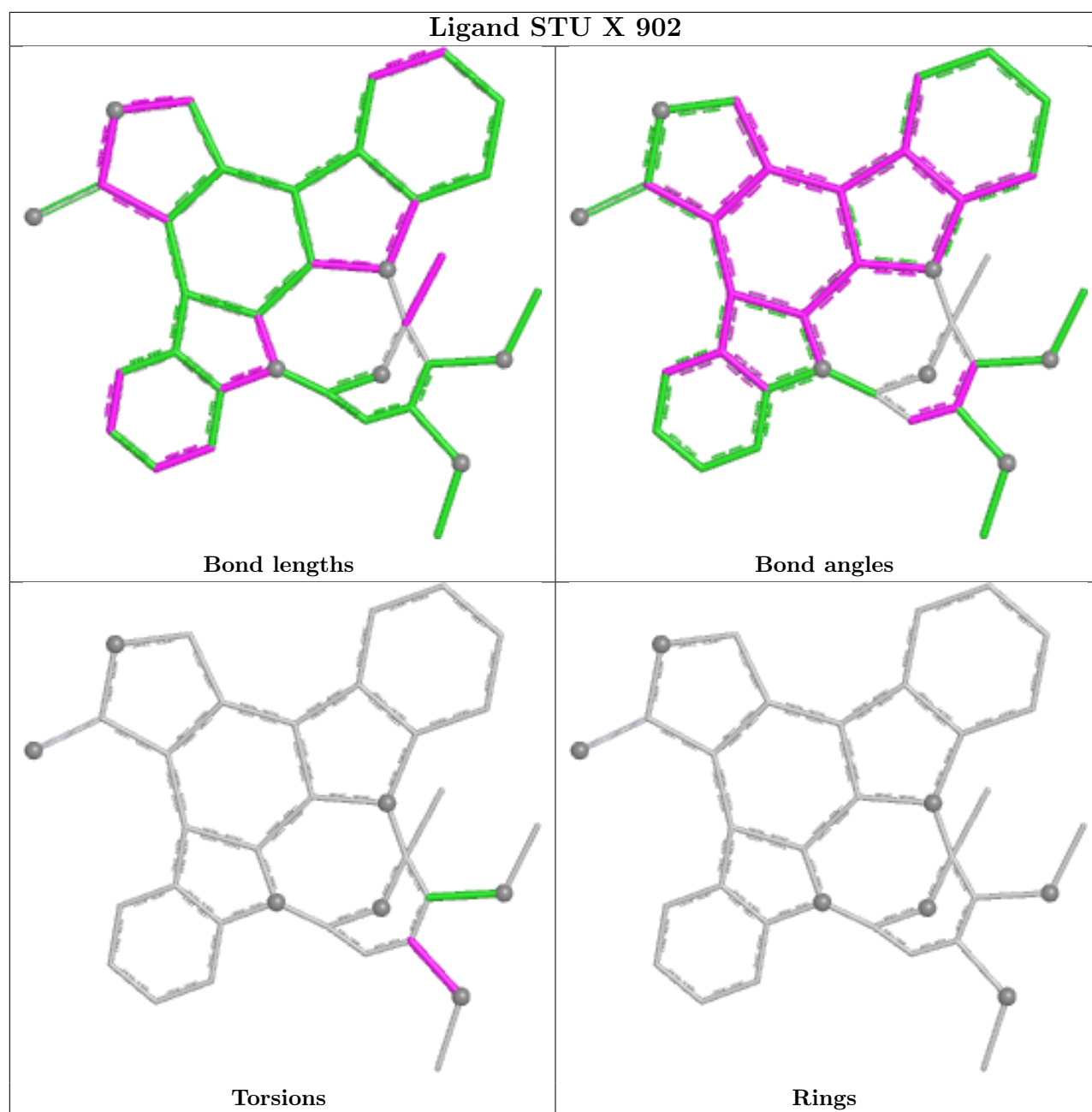
Mol	Chain	Res	Type	Atoms
2	X	902	STU	C24-C23-N4-C28

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	902	STU	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	X	262/283 (92%)	0.47	14 (5%) 32 24	18, 39, 75, 123	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	223	TYR	4.3
1	X	218	GLN	4.0
1	X	166	ALA	3.5
1	X	162	ALA	3.4
1	X	263	TYR	2.9
1	X	157	ASP	2.8
1	X	245	LYS	2.7
1	X	156	GLU	2.6
1	X	21	GLN	2.6
1	X	158	ASN	2.5
1	X	230	ASP	2.5
1	X	168	PHE	2.3
1	X	64	ASP	2.3
1	X	165	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	PTR	X	160	16/17	0.73	0.19	114,122,130,130	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

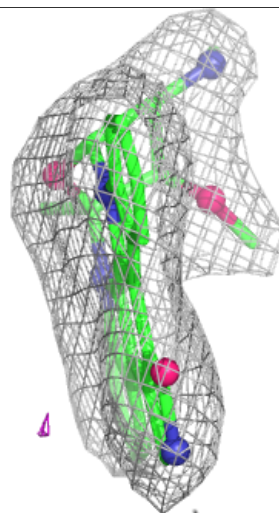
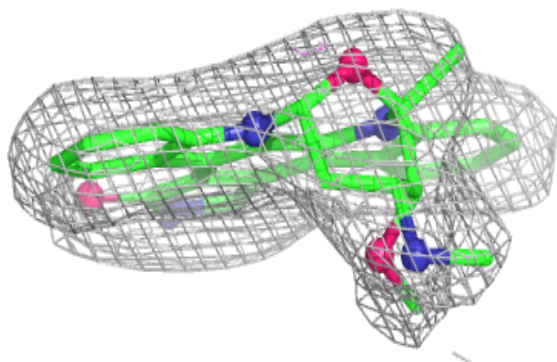
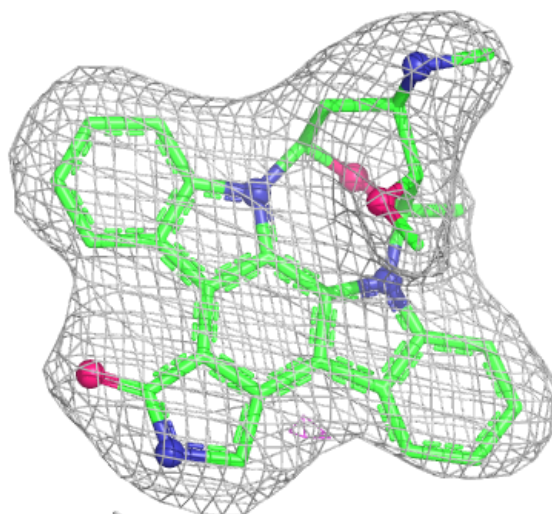
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	STU	X	902	35/35	0.95	0.08	14,21,25,27	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 STU X 902:

$2mF_o-DF_c$ (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.