Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 08:13 AM EDT

PDB ID	:	3CBL
Title	:	Crystal structure of human feline sarcoma viral oncogene homologue (v-FES) in complex with staurosporine and a consensus peptide
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Deposited on	:	2008-02-22
Resolution	:	1.75 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 (i) 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 (1)) were used in the production of this report:

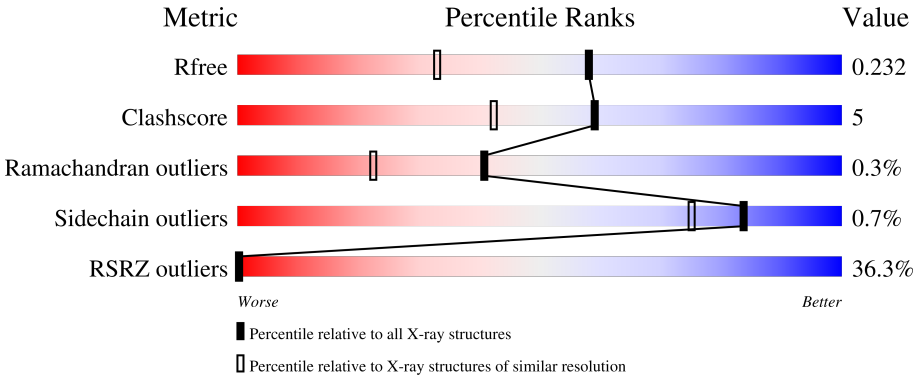
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	377	35%, 86%, 8%, 6%
2	B	6	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3304 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 Fes/Fps.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	2824	1815	479	515	15	0	13	0

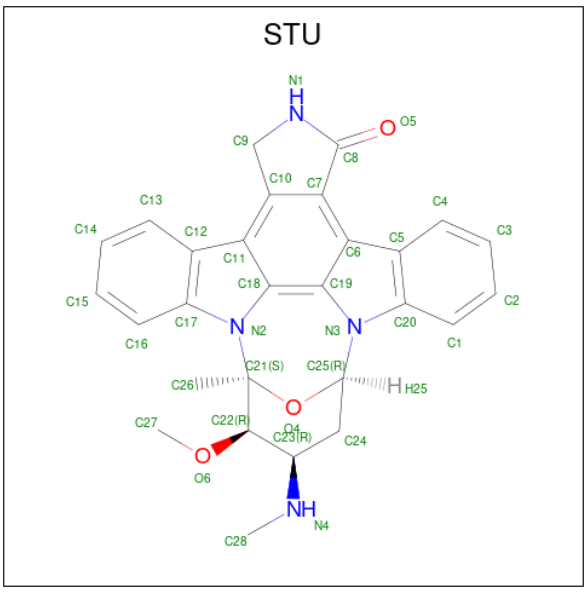
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	SER	-	expression tag	UNP P07332
A	447	MET	-	expression tag	UNP P07332

- Molecule 2 is a protein called Synthetic peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	47	31	5	11	0	0	0

- Molecule 3 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



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

- Molecule 4 is water.

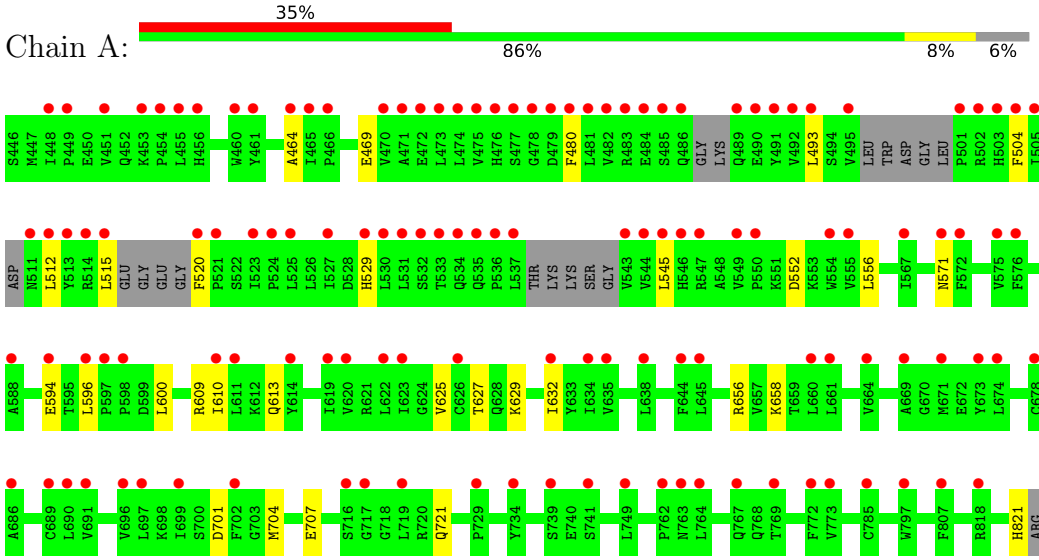
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	320	Total	O	0	0
			320	320		
4	B	8	Total	O	0	0
			8	8		

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.

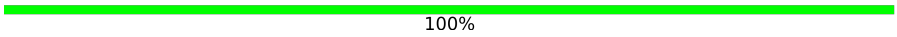
• Molecule 1: Proto-oncogene tyrosine-protein kinase Fes/Fps

Chain A:



• Molecule 2: Synthetic peptide

Chain B:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	35.68Å 77.18Å 149.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.58 – 1.75 38.59 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.58-1.75) 99.1 (38.59-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.227 0.187 , 0.232	Depositor DCC
R_{free} test set	2141 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3304	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ACE, 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	A	0.68	0/2935	0.73	2/3977 (0.1%)
2	B	0.78	0/45	0.81	0/59
All	All	0.68	0/2980	0.73	2/4036 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	556	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	552	ASP	CB-CG-OD1	5.30	123.07	118.30

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	2824	0	2778	22	0
2	B	47	0	45	0	0
3	A	105	0	78	6	0
4	A	320	0	0	2	0
4	B	8	0	0	1	0
All	All	3304	0	2901	28	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 (28) 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)
3:A:902:STU:H261	3:A:902:STU:H16	1.63	0.81
1:A:627:THR:HA	1:A:632:ILE:HD12	1.62	0.80
1:A:704[A]:MET:HE2	4:A:321:HOH:O	1.87	0.74
3:A:903:STU:H261	3:A:903:STU:H16	1.74	0.68
1:A:704[A]:MET:CE	4:A:321:HOH:O	2.44	0.63
1:A:480:PHE:CG	1:A:545:LEU:HD22	2.34	0.63
3:A:901:STU:H261	3:A:901:STU:H16	1.80	0.63
1:A:625:VAL:HG12	1:A:627:THR:HG23	1.81	0.62
1:A:721:GLN:HG2	4:B:169:HOH:O	2.03	0.59
1:A:493:LEU:HD23	1:A:515:LEU:HD11	1.84	0.59
1:A:629:LYS:O	1:A:632:ILE:HD13	2.03	0.58
1:A:464:ALA:HB3	1:A:632:ILE:HD11	1.88	0.55
1:A:469:GLU:OE1	1:A:609:ARG:NH2	2.40	0.54
3:A:902:STU:H16	3:A:902:STU:C26	2.38	0.53
1:A:493:LEU:CD2	1:A:515:LEU:HD11	2.40	0.51
1:A:504:PHE:HB3	1:A:515:LEU:HD22	1.92	0.50
1:A:480:PHE:CD1	1:A:545:LEU:HD22	2.47	0.49
1:A:579:ARG:HG2	1:A:586:LEU:HD23	1.95	0.49
1:A:571[B]:ASN:ND2	1:A:721:GLN:HE22	2.13	0.46
1:A:512:LEU:HD23	1:A:520:PHE:C	2.36	0.46
1:A:613:GLN:NE2	1:A:707[B]:GLU:OE2	2.38	0.46
1:A:520:PHE:CZ	1:A:529:HIS:CB	2.99	0.45
1:A:656:ARG:HD3	1:A:658:LYS:HZ3	1.83	0.44
3:A:903:STU:H16	3:A:903:STU:C26	2.45	0.42
3:A:902:STU:C26	3:A:902:STU:C16	2.98	0.41
1:A:610:ILE:CD1	1:A:707[B]:GLU:HG3	2.51	0.41
1:A:596:LEU:HD22	1:A:600:LEU:HD23	2.02	0.41
1:A:464:ALA:CB	1:A:632:ILE:HD11	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	357/377 (95%)	349 (98%)	7 (2%)	1 (0%)	41 22
2	B	4/6 (67%)	4 (100%)	0	0	100 100
All	All	361/383 (94%)	353 (98%)	7 (2%)	1 (0%)	41 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	701	ASP

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	305/327 (93%)	303 (99%)	2 (1%)	84 75
2	B	5/5 (100%)	5 (100%)	0	100 100
All	All	310/332 (93%)	308 (99%)	2 (1%)	84 79

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	594	GLU
1	A	821	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are 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	$\#\|Z\| > 2$
3	STU	A	902	-	30,42,42	1.52	6 (20%)	31,68,68	2.20	9 (29%)
3	STU	A	903	-	30,42,42	1.90	6 (20%)	31,68,68	1.79	9 (29%)
3	STU	A	901	-	30,42,42	1.75	8 (26%)	31,68,68	1.28	5 (16%)

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	STU	A	902	-	-	0/4/42/42	-
3	STU	A	903	-	-	1/4/42/42	-
3	STU	A	901	-	-	0/4/42/42	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	STU	C7-C8	-5.30	1.40	1.49
3	A	901	STU	C7-C8	-4.97	1.41	1.49
3	A	903	STU	C8-N1	-4.78	1.31	1.35
3	A	902	STU	C7-C8	-4.42	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	STU	C24-C25	3.56	1.58	1.51
3	A	903	STU	C26-C21	3.16	1.55	1.51
3	A	902	STU	C11-C18	-2.59	1.39	1.42
3	A	901	STU	C6-C19	-2.51	1.39	1.42
3	A	901	STU	C8-N1	-2.44	1.33	1.35
3	A	901	STU	C3-C4	2.42	1.42	1.36
3	A	901	STU	C24-C25	2.41	1.56	1.51
3	A	902	STU	C9-N1	2.35	1.48	1.45
3	A	903	STU	C11-C18	-2.32	1.39	1.42
3	A	903	STU	C9-C10	2.29	1.52	1.50
3	A	901	STU	C9-C10	2.20	1.52	1.50
3	A	902	STU	C8-N1	-2.19	1.33	1.35
3	A	901	STU	C7-C6	-2.18	1.39	1.43
3	A	902	STU	C22-C23	2.17	1.55	1.52
3	A	902	STU	C3-C4	2.06	1.41	1.36
3	A	901	STU	C26-C21	2.05	1.54	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	STU	C7-C8-N1	5.40	111.84	106.37
3	A	902	STU	C9-N1-C8	-5.39	108.67	113.85
3	A	903	STU	O5-C8-N1	-5.27	119.11	125.27
3	A	903	STU	C7-C8-N1	4.66	111.08	106.37
3	A	902	STU	O5-C8-N1	-4.60	119.90	125.27
3	A	902	STU	O4-C25-C24	4.13	118.28	112.31
3	A	902	STU	C26-C21-C22	-3.51	105.81	112.64
3	A	901	STU	C7-C8-N1	3.42	109.83	106.37
3	A	903	STU	C6-C7-C8	2.98	134.21	129.76
3	A	902	STU	O5-C8-C7	-2.79	126.01	129.32
3	A	901	STU	O5-C8-C7	-2.61	126.22	129.32
3	A	903	STU	C9-N1-C8	-2.48	111.46	113.85
3	A	902	STU	C6-C7-C8	2.47	133.46	129.76
3	A	901	STU	C6-C7-C8	2.44	133.40	129.76
3	A	903	STU	C26-C21-C22	-2.43	107.90	112.64
3	A	903	STU	C1-C20-N3	-2.21	129.61	132.25
3	A	903	STU	C16-C17-C12	-2.11	117.69	120.73
3	A	902	STU	C27-O6-C22	2.10	118.06	114.44
3	A	903	STU	C27-O6-C22	-2.09	110.84	114.44
3	A	901	STU	C16-C17-C12	-2.08	117.73	120.73
3	A	903	STU	C15-C14-C13	-2.06	117.55	120.44
3	A	901	STU	C26-C21-C22	-2.01	108.73	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	STU	C16-C17-C12	-2.00	117.84	120.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	STU	C24-C23-N4-C28

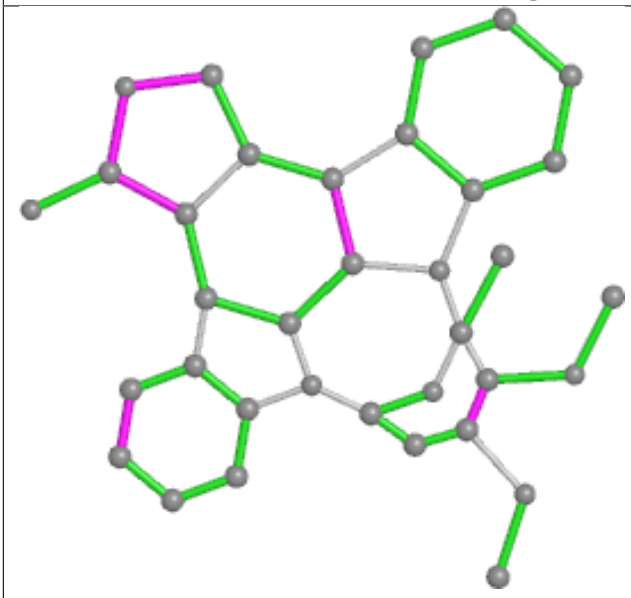
There are no ring outliers.

3 monomers are involved in 6 short contacts:

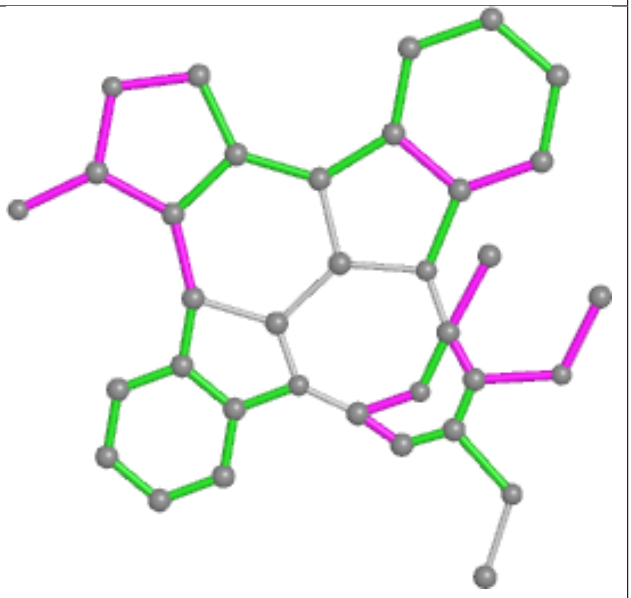
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	STU	3	0
3	A	903	STU	2	0
3	A	901	STU	1	0

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 then 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.

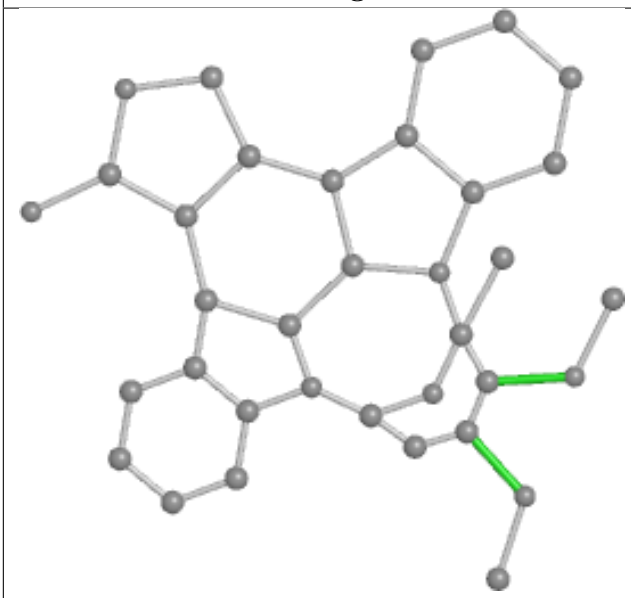
Ligand STU A 902



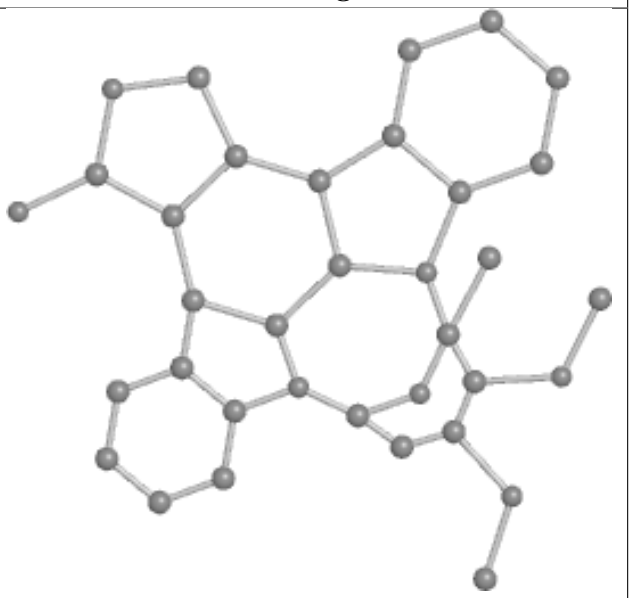
Bond lengths



Bond angles

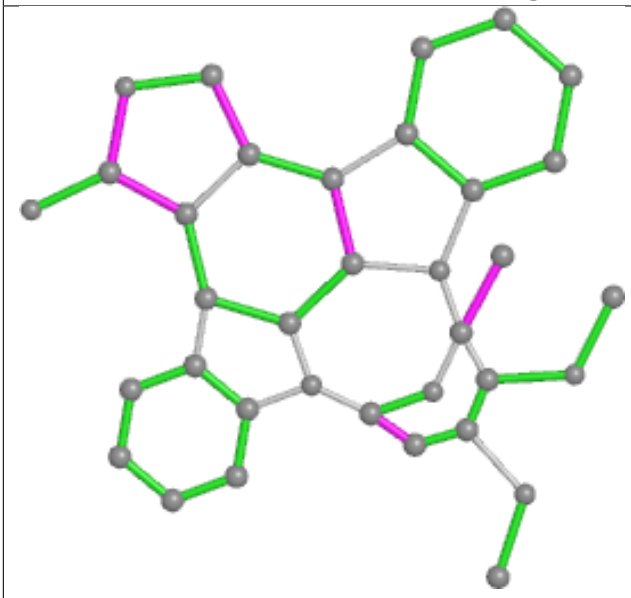


Torsions

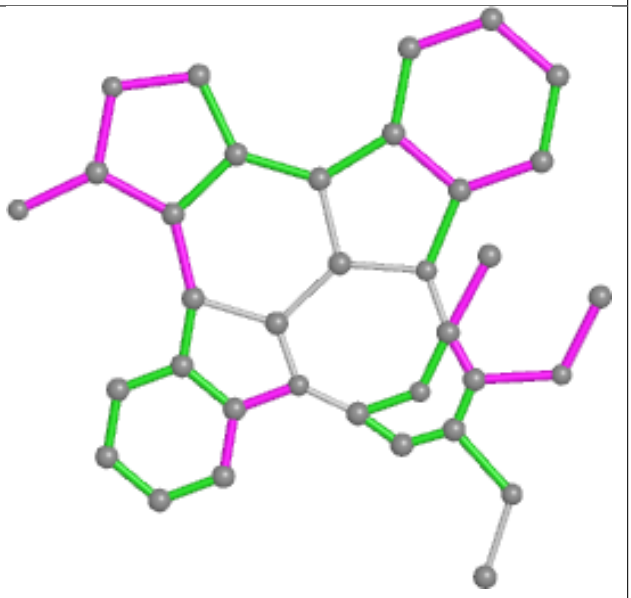


Rings

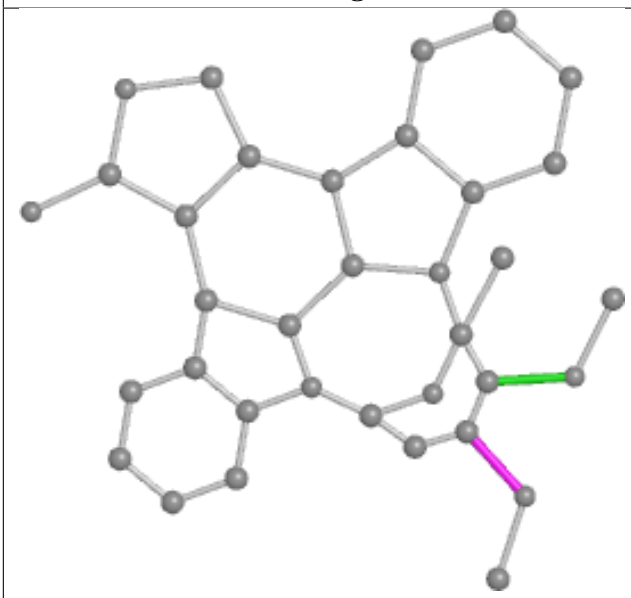
Ligand STU A 903



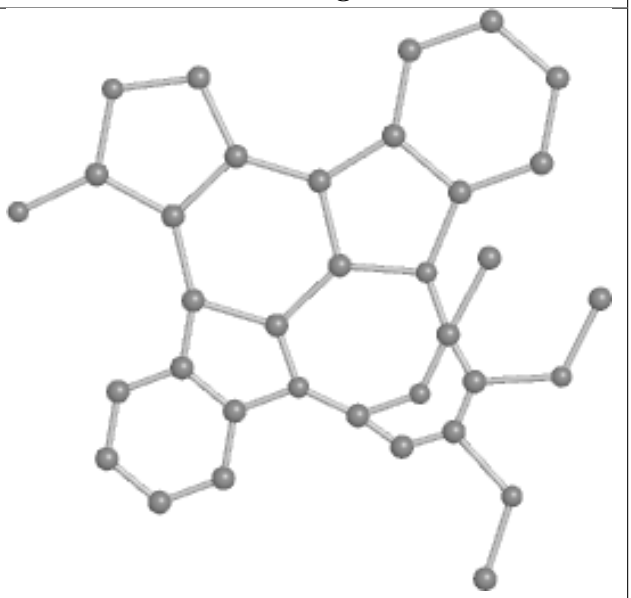
Bond lengths



Bond angles

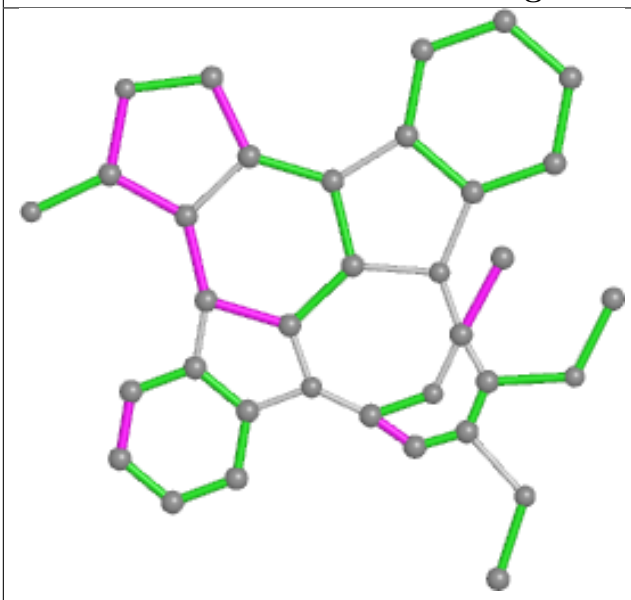


Torsions

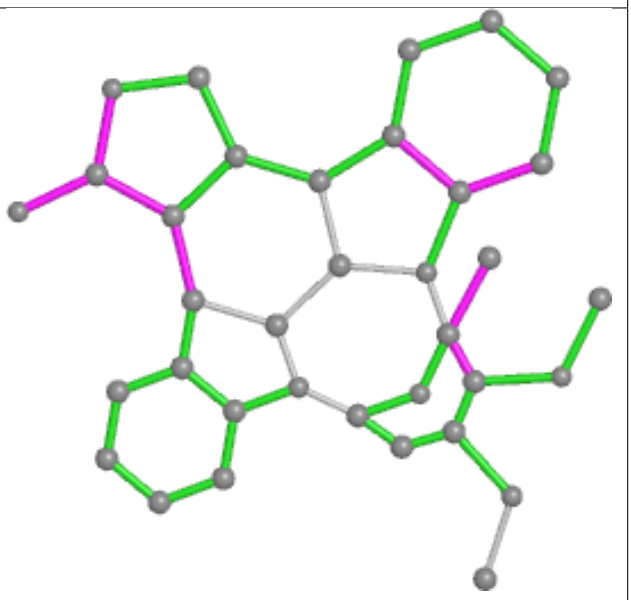


Rings

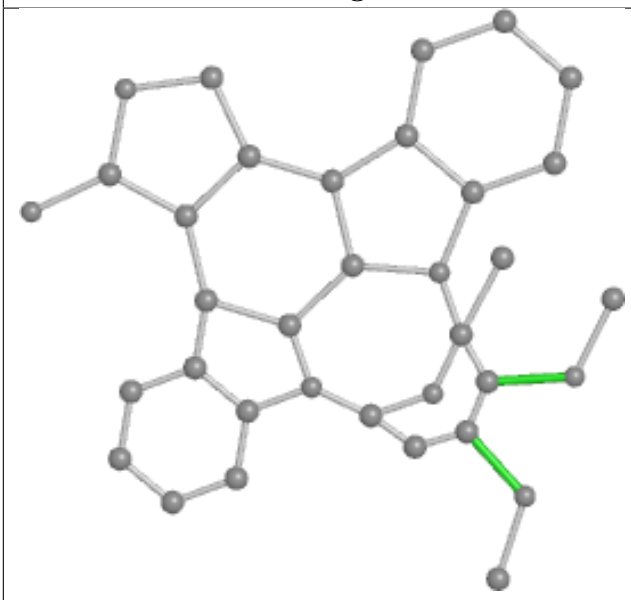
Ligand STU A 901



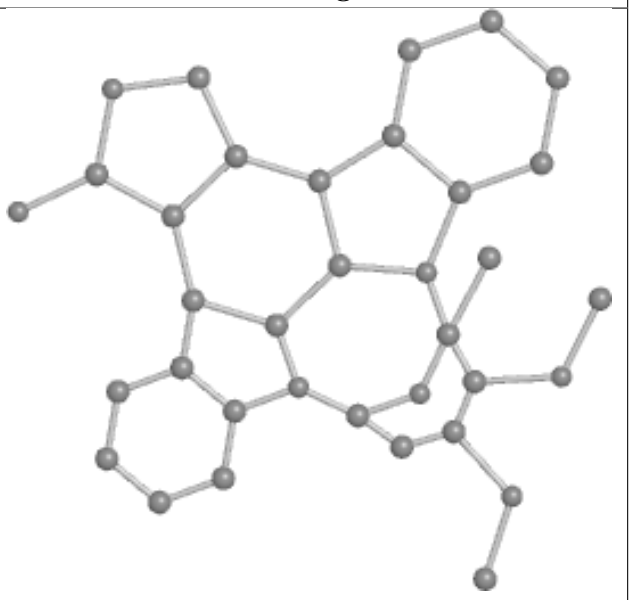
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	356/377 (94%)	2.13	131 (36%) 0 0	24, 37, 52, 63	0
2	B	5/6 (83%)	0.17	0 100 100	31, 32, 38, 51	0
All	All	361/383 (94%)	2.11	131 (36%) 0 0	24, 37, 52, 63	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	LEU	11.0
1	A	536	PRO	10.3
1	A	513	TYR	9.0
1	A	473	LEU	8.4
1	A	471	ALA	8.4
1	A	495	VAL	8.1
1	A	478	GLY	7.7
1	A	544	VAL	7.6
1	A	480	PHE	7.4
1	A	537	LEU	7.2
1	A	474	LEU	7.0
1	A	515	LEU	6.8
1	A	546	HIS	6.6
1	A	477	SER	6.4
1	A	543	VAL	6.4
1	A	506	ILE	6.4
1	A	533	THR	6.3
1	A	470	VAL	6.3
1	A	460	TRP	6.3
1	A	530	LEU	6.2
1	A	520	PHE	6.0
1	A	549	VAL	6.0
1	A	531	LEU	5.8
1	A	511	ASN	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	529	HIS	5.4
1	A	493	LEU	5.3
1	A	504	PHE	5.3
1	A	535	GLN	5.2
1	A	489	GLN	5.1
1	A	523	ILE	5.0
1	A	532	SER	5.0
1	A	521	PRO	4.9
1	A	454	PRO	4.9
1	A	475	VAL	4.8
1	A	479	ASP	4.7
1	A	545	LEU	4.7
1	A	482	VAL	4.5
1	A	503	HIS	4.3
1	A	716	SER	4.2
1	A	505	ILE	4.2
1	A	501	PRO	3.9
1	A	485	SER	3.9
1	A	527	ILE	3.8
1	A	456	HIS	3.8
1	A	764	LEU	3.8
1	A	717	GLY	3.7
1	A	465	ILE	3.7
1	A	491	TYR	3.7
1	A	534	GLN	3.6
1	A	767	GLN	3.6
1	A	476	HIS	3.6
1	A	678	CYS	3.6
1	A	679	CYS	3.5
1	A	525	LEU	3.3
1	A	492	VAL	3.3
1	A	455	LEU	3.3
1	A	514	ARG	3.3
1	A	620	VAL	3.3
1	A	524	PRO	3.2
1	A	571[A]	ASN	3.2
1	A	699[A]	ILE	3.1
1	A	483	ARG	3.1
1	A	486	GLN	3.1
1	A	702	PHE	3.1
1	A	684	LEU	3.1
1	A	691	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	596	LEU	3.0
1	A	690	LEU	3.0
1	A	773	VAL	3.0
1	A	547	ARG	3.0
1	A	461	TYR	3.0
1	A	611	LEU	2.9
1	A	490	GLU	2.9
1	A	674	LEU	2.8
1	A	772	PHE	2.8
1	A	597	PRO	2.8
1	A	686	ALA	2.8
1	A	689	CYS	2.7
1	A	449	PRO	2.7
1	A	466	PRO	2.7
1	A	634	ILE	2.7
1	A	661	LEU	2.7
1	A	719	LEU	2.6
1	A	763	ASN	2.6
1	A	623[A]	ILE	2.6
1	A	567	ILE	2.6
1	A	619	ILE	2.5
1	A	484	GLU	2.5
1	A	448	ILE	2.5
1	A	575	VAL	2.5
1	A	638	LEU	2.4
1	A	554	TRP	2.4
1	A	739[A]	SER	2.4
1	A	588	ALA	2.4
1	A	572	PHE	2.4
1	A	635	VAL	2.3
1	A	818[A]	ARG	2.3
1	A	610	ILE	2.3
1	A	576	PHE	2.3
1	A	594	GLU	2.3
1	A	769	THR	2.3
1	A	451[A]	VAL	2.3
1	A	453	LYS	2.3
1	A	696	VAL	2.3
1	A	472	GLU	2.3
1	A	632	ILE	2.3
1	A	671	MET	2.3
1	A	622	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	749	LEU	2.2
1	A	741[A]	SER	2.2
1	A	807	PHE	2.2
1	A	785	CYS	2.2
1	A	660	LEU	2.2
1	A	797	TRP	2.2
1	A	626	CYS	2.2
1	A	464	ALA	2.2
1	A	669	ALA	2.2
1	A	502	ARG	2.1
1	A	481	LEU	2.1
1	A	645	LEU	2.1
1	A	550	PRO	2.1
1	A	644	PHE	2.1
1	A	673	TYR	2.1
1	A	729	PRO	2.0
1	A	555	VAL	2.0
1	A	762	PRO	2.0
1	A	614	TYR	2.0
1	A	734	TYR	2.0
1	A	664	VAL	2.0
1	A	697	LEU	2.0
1	A	598	PRO	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 monosaccharides 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, 95^{th} 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.

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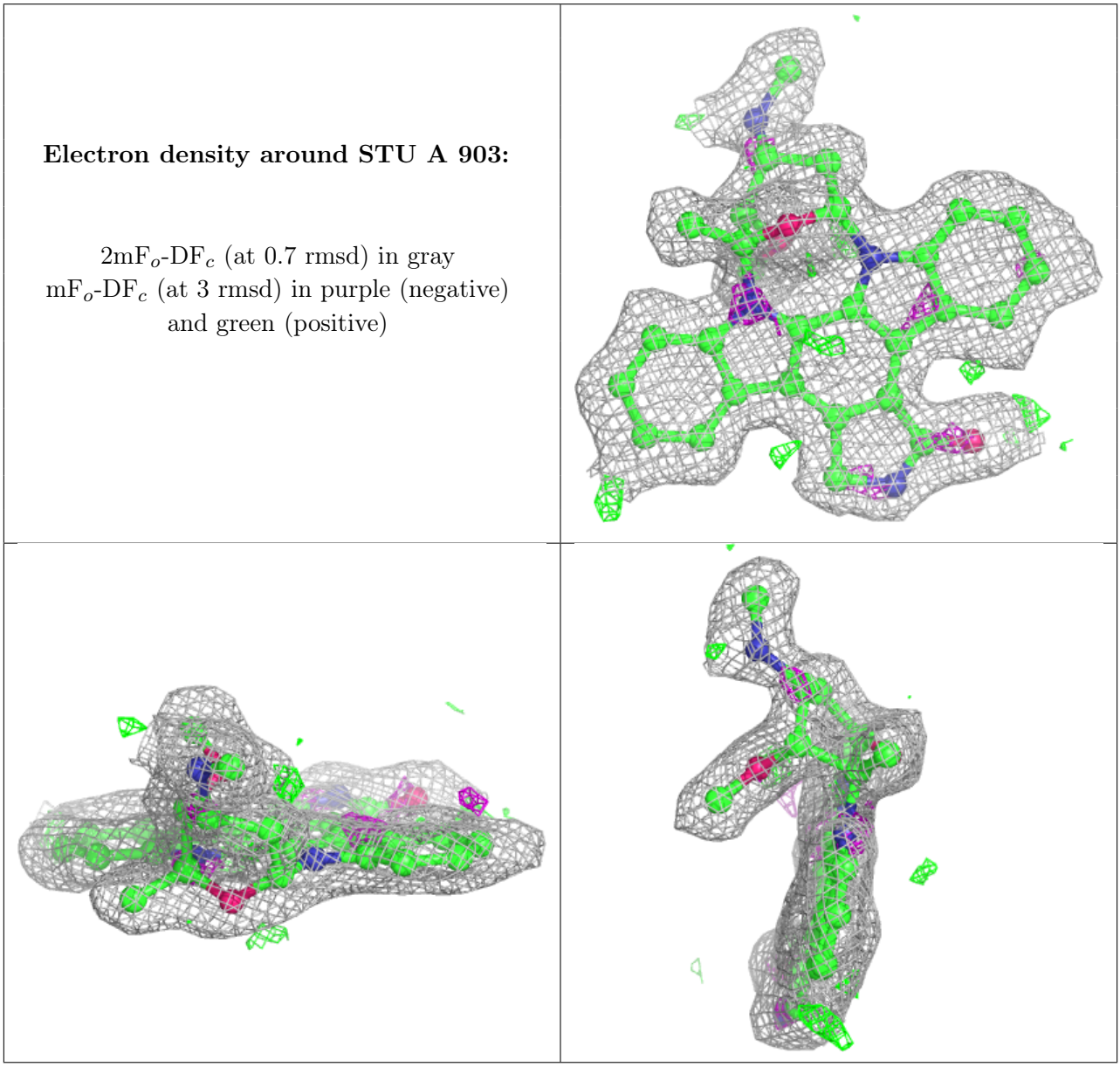
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	STU	A	903	35/35	0.82	0.19	30,35,43,47	0
3	STU	A	902	35/35	0.89	0.16	24,30,34,38	0
3	STU	A	901	35/35	0.93	0.11	18,22,27,36	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.

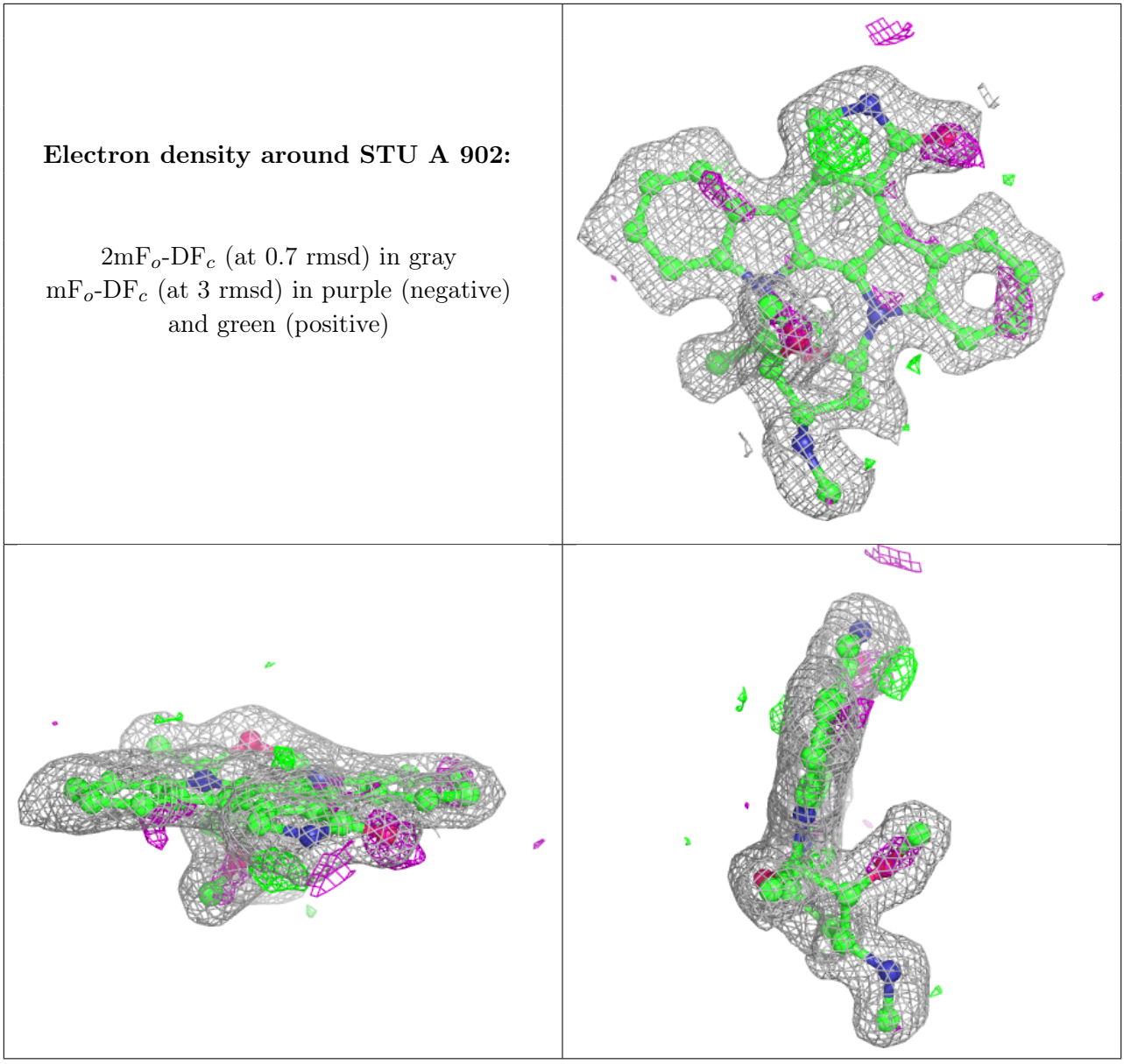
Electron density around STU A 903:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



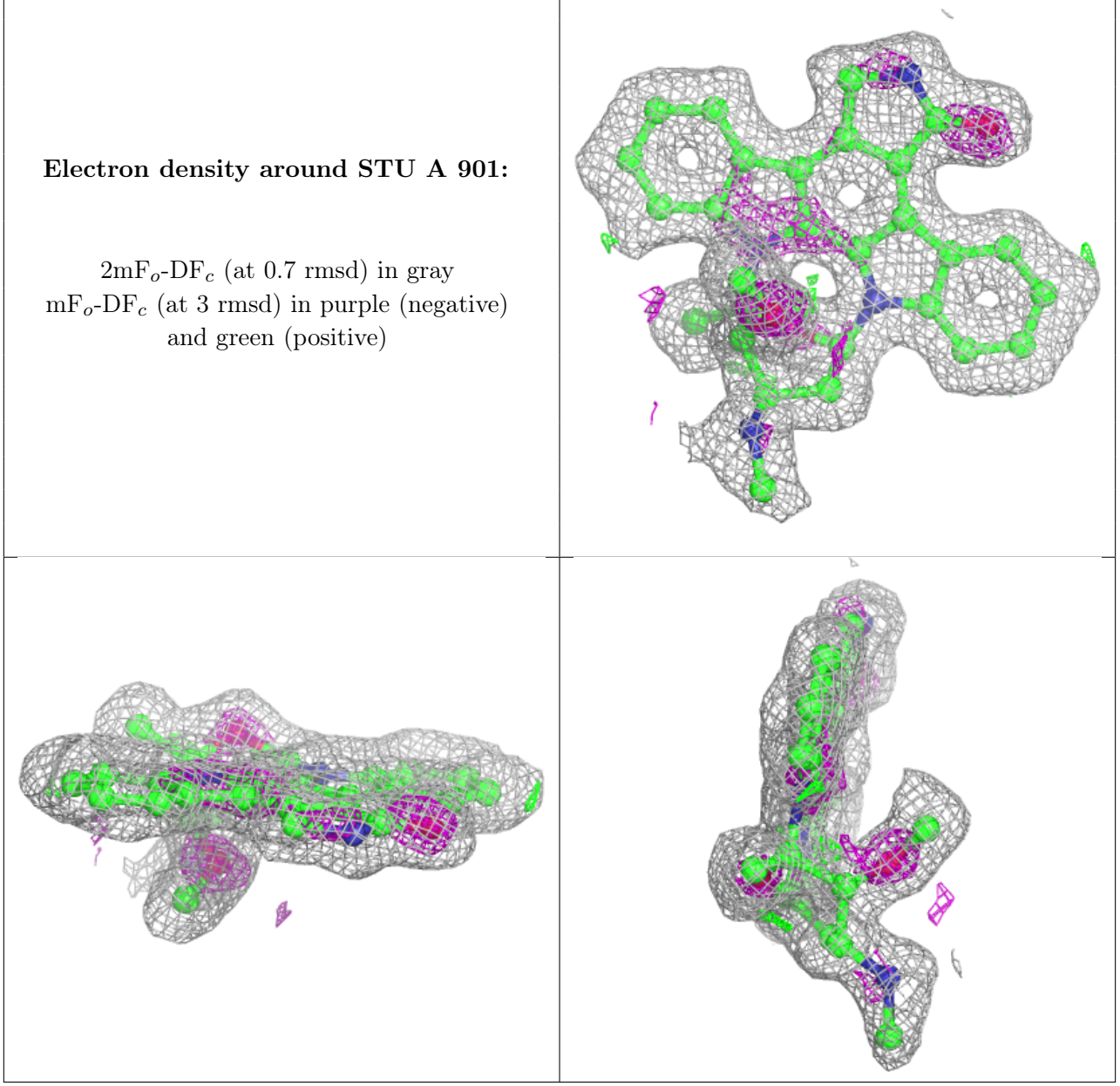
Electron density around STU A 902:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around STU A 901:

$2mF_o$-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.