Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 08:39 AM EDT

PDB ID	:	3CD3
Title	:	Crystal structure of phosphorylated human feline sarcoma viral oncogene homologue (v-FES) in complex with staurosporine and a consensus peptide
Authors	:	Filippakopoulos, P.; Salah, E.; Cooper, C.; Picaud, S.S.; Elkins, J.M.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on	:	2008-02-26
Resolution	:	1.98 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 (i)) were used in the production of this report:

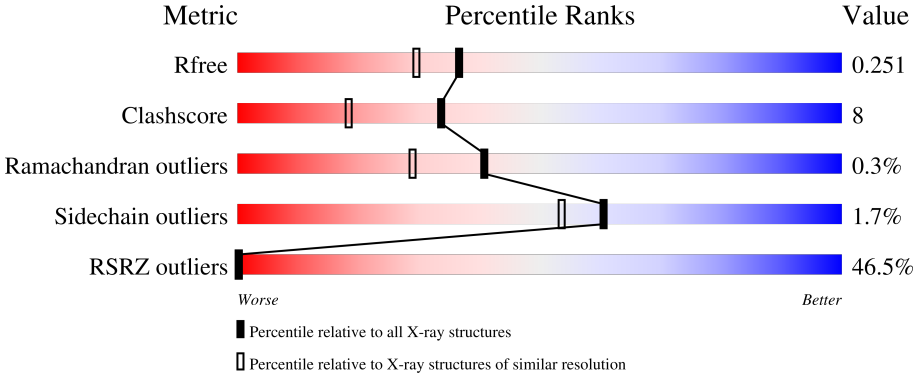
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	44% 80% 14% • 6%
2	B	6	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3232 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	P	S			
1	A	353	2771	1777	477	502	1	14	0	9	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

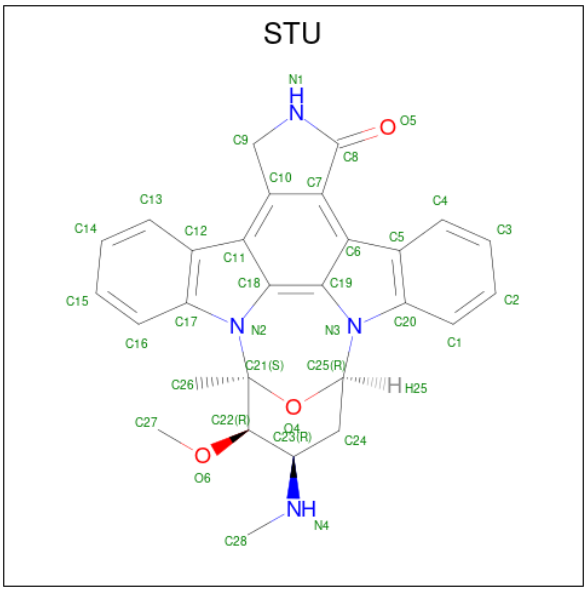
- Molecule 2 is a protein called Synthetic peptide.

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	2	2	2	0	0

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



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

- Molecule 5 is water.

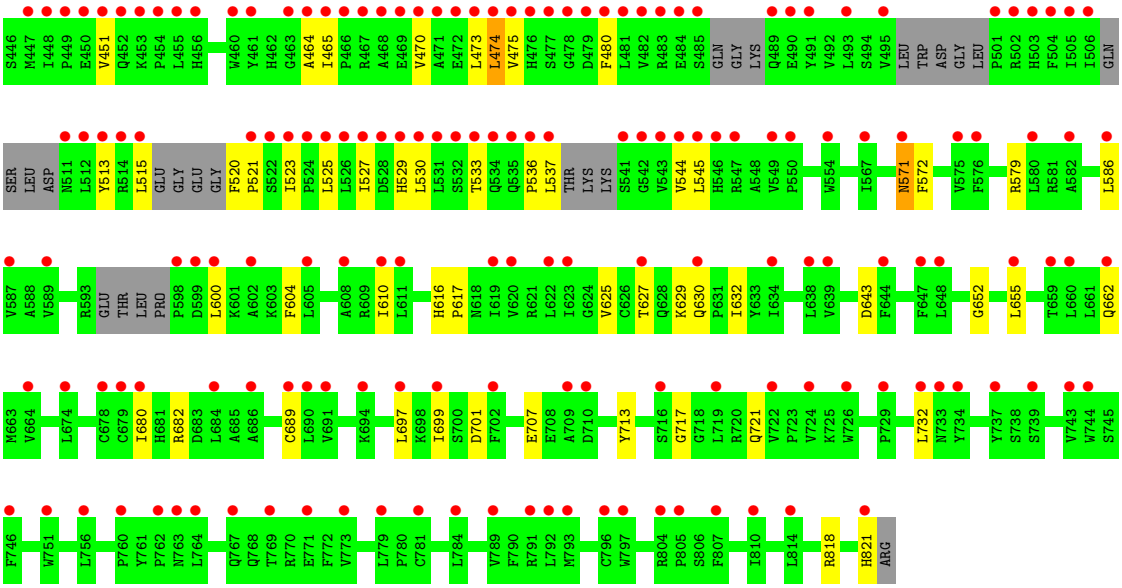
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	299	299	299	0	0
			Total	O		
5	B	8	8	8	0	0

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.

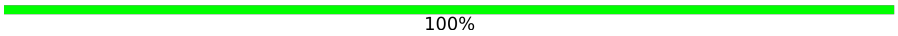
• Molecule 1: Proto-oncogene tyrosine-protein kinase Fes/Fps

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	35.45Å 76.91Å 150.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.35 – 1.98 14.95 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.35-1.98) 97.6 (14.95-1.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.98Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.247 0.199 , 0.251	Depositor DCC
R_{free} test set	1447 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3232	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, STU, PTR, ACE

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	0/2854	0.74	0/3863
2	B	0.81	0/45	0.89	0/59
All	All	0.68	0/2899	0.74	0/3922

There are no bond length outliers.

There are no bond angle outliers.

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	A	2771	0	2699	40	0
2	B	47	0	45	0	0
3	A	2	0	0	0	0
4	A	105	0	78	9	0
5	A	299	0	0	2	0
5	B	8	0	0	1	0
All	All	3232	0	2822	49	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 8.

All (49) 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:627:THR:HA	1:A:632:ILE:HD12	1.56	0.86
4:A:903:STU:H261	4:A:903:STU:H16	1.57	0.85
4:A:902:STU:H261	4:A:902:STU:H16	1.65	0.77
4:A:901:STU:H261	4:A:901:STU:H16	1.69	0.74
1:A:717:GLY:O	5:A:310:HOH:O	2.05	0.73
1:A:610:ILE:CD1	1:A:707[B]:GLU:HG3	2.29	0.63
1:A:625:VAL:HG12	1:A:627:THR:HG23	1.81	0.62
1:A:721:GLN:HG3	5:B:165:HOH:O	1.99	0.62
1:A:465:ILE:HD11	1:A:473:LEU:CD1	2.30	0.61
4:A:903:STU:H16	4:A:903:STU:C26	2.31	0.59
1:A:689:CYS:SG	1:A:699[A]:ILE:HD12	2.44	0.58
1:A:610:ILE:HD13	1:A:707[B]:GLU:HG3	1.86	0.57
1:A:465:ILE:HD11	1:A:473:LEU:HD12	1.87	0.56
1:A:530:LEU:HD13	1:A:537:LEU:CD2	2.35	0.56
1:A:610:ILE:HD13	1:A:707[B]:GLU:CG	2.36	0.55
1:A:610:ILE:HD13	1:A:707[B]:GLU:OE1	2.07	0.55
1:A:465:ILE:O	1:A:465:ILE:HG23	2.07	0.54
4:A:903:STU:H261	4:A:903:STU:C16	2.35	0.54
1:A:627:THR:HA	1:A:632:ILE:CD1	2.36	0.52
1:A:464:ALA:HB1	1:A:630:GLN:HE21	1.75	0.51
1:A:579:ARG:HG2	1:A:586:LEU:HD23	1.94	0.50
4:A:901:STU:H273	4:A:901:STU:C17	2.42	0.49
1:A:697:LEU:HD21	1:A:699[A]:ILE:CD1	2.42	0.49
1:A:652:GLY:HA2	1:A:655:LEU:HD12	1.95	0.48
1:A:662:GLN:HB2	1:A:818:ARG:NE	2.29	0.48
1:A:523:ILE:O	1:A:527:ILE:HG12	2.13	0.47
1:A:604:PHE:HE2	1:A:632:ILE:HG22	1.78	0.47
1:A:480:PHE:CG	1:A:545:LEU:HD22	2.49	0.47
1:A:465:ILE:HD11	1:A:473:LEU:HD11	1.96	0.47
4:A:903:STU:C26	4:A:903:STU:C16	2.91	0.47
1:A:470:VAL:HG12	1:A:474:LEU:HD22	1.96	0.46
1:A:697:LEU:C	1:A:697:LEU:HD23	2.36	0.46
1:A:529:HIS:CE1	1:A:533:THR:HG21	2.50	0.46
1:A:515:LEU:CD1	1:A:537:LEU:HD22	2.46	0.46
1:A:572:PHE:CE1	1:A:600:LEU:HG	2.51	0.46
1:A:629:LYS:HD2	5:A:332:HOH:O	2.17	0.45
1:A:536:PRO:HA	1:A:544:VAL:HG22	1.99	0.45
1:A:513:TYR:O	1:A:520:PHE:N	2.51	0.44
1:A:451:VAL:HG12	1:A:451:VAL:O	2.18	0.43
1:A:616:HIS:CG	1:A:617:PRO:HD2	2.53	0.43
1:A:521:PRO:HD2	1:A:525:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ILE:O	1:A:465:ILE:CG2	2.67	0.42
1:A:732:LEU:HD23	1:A:732:LEU:C	2.41	0.41
4:A:902:STU:H261	4:A:902:STU:C16	2.42	0.41
1:A:464:ALA:HB3	1:A:632:ILE:HD11	2.03	0.41
4:A:901:STU:H16	4:A:901:STU:C26	2.43	0.40
1:A:680:ILE:HG22	1:A:682:ARG:HG3	2.04	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	347/377 (92%)	338 (97%)	8 (2%)	1 (0%)	41	29
2	B	4/6 (67%)	4 (100%)	0	0	100	100
All	All	351/383 (92%)	342 (97%)	8 (2%)	1 (0%)	41	29

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	293/326 (90%)	287 (98%)	6 (2%)	55	48
2	B	5/5 (100%)	5 (100%)	0	100	100
All	All	298/331 (90%)	292 (98%)	6 (2%)	60	48

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	474	LEU
1	A	475	VAL
1	A	571[A]	ASN
1	A	571[B]	ASN
1	A	643	ASP
1	A	821	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	529	HIS
1	A	630	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	A	713	1	15,16,17	2.10	1 (6%)	19,22,24	1.07	1 (5%)

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	A	713	1	-	0/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	713	PTR	OH-CZ	-7.70	1.23	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	713	PTR	OH-CZ-CE2	2.23	125.86	119.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	STU	A	902	-	30,42,42	2.09	8 (26%)	31,68,68	2.17	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	STU	A	903	-	30,42,42	2.18	8 (26%)	31,68,68	2.29	7 (22%)
4	STU	A	901	-	30,42,42	2.14	7 (23%)	31,68,68	1.95	6 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	STU	A	902	-	-	0/4/42/42	-
4	STU	A	903	-	-	1/4/42/42	-
4	STU	A	901	-	-	1/4/42/42	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	STU	C9-C10	6.74	1.55	1.50
4	A	901	STU	C7-C8	-5.75	1.40	1.49
4	A	903	STU	C9-C10	5.20	1.54	1.50
4	A	902	STU	C7-C8	-5.13	1.41	1.49
4	A	903	STU	C7-C8	-4.99	1.41	1.49
4	A	901	STU	O6-C22	4.64	1.50	1.42
4	A	902	STU	C8-N1	-4.56	1.31	1.35
4	A	903	STU	O6-C22	4.28	1.49	1.42
4	A	902	STU	O6-C22	3.86	1.49	1.42
4	A	903	STU	O4-C25	3.53	1.49	1.43
4	A	902	STU	C9-N1	3.49	1.49	1.45
4	A	903	STU	C24-C25	3.32	1.58	1.51
4	A	903	STU	C11-C18	-3.30	1.38	1.42
4	A	902	STU	C11-C18	-3.24	1.38	1.42
4	A	902	STU	C22-C23	3.08	1.56	1.52
4	A	903	STU	C8-N1	-3.04	1.32	1.35
4	A	902	STU	C26-C21	3.03	1.55	1.51
4	A	901	STU	C24-C25	2.72	1.57	1.51
4	A	903	STU	C10-C11	-2.31	1.39	1.42
4	A	901	STU	C15-C16	2.22	1.41	1.36
4	A	901	STU	C10-C11	-2.14	1.39	1.42
4	A	901	STU	C6-C19	-2.09	1.40	1.42
4	A	902	STU	C6-C19	-2.07	1.40	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	903	STU	C7-C8-N1	7.23	113.69	106.37
4	A	901	STU	C7-C8-N1	6.89	113.34	106.37
4	A	902	STU	C7-C8-N1	6.09	112.53	106.37
4	A	902	STU	O5-C8-N1	-5.90	118.38	125.27
4	A	903	STU	O5-C8-N1	-5.85	118.43	125.27
4	A	903	STU	C6-C7-C8	4.14	135.95	129.76
4	A	902	STU	C9-N1-C8	-4.07	109.94	113.85
4	A	903	STU	C9-N1-C8	-3.99	110.02	113.85
4	A	901	STU	O5-C8-C7	-3.93	124.65	129.32
4	A	902	STU	C6-C7-C8	3.86	135.53	129.76
4	A	901	STU	C9-N1-C8	-3.80	110.19	113.85
4	A	903	STU	O4-C25-C24	3.63	117.55	112.31
4	A	901	STU	C26-C21-C22	-3.16	106.48	112.64
4	A	903	STU	O5-C8-C7	-3.03	125.73	129.32
4	A	901	STU	O5-C8-N1	-2.91	121.87	125.27
4	A	902	STU	O4-C25-C24	2.68	116.19	112.31
4	A	901	STU	C6-C7-C8	2.66	133.74	129.76
4	A	902	STU	C1-C20-N3	-2.61	129.13	132.25
4	A	903	STU	C26-C21-C22	-2.30	108.16	112.64
4	A	902	STU	C16-C17-C12	-2.21	117.54	120.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	903	STU	C24-C23-N4-C28
4	A	901	STU	C21-C22-O6-C27

There are no ring outliers.

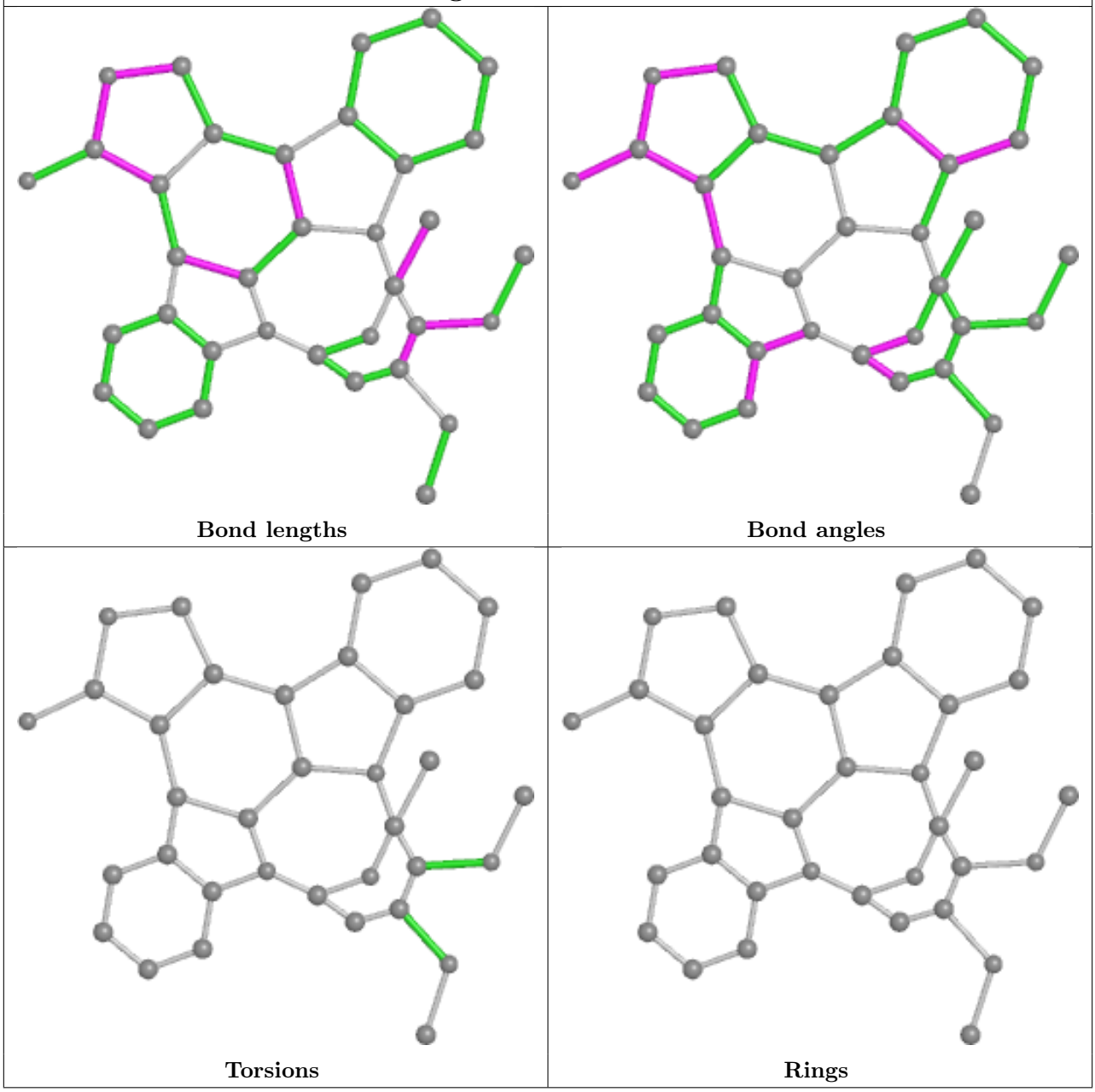
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	STU	2	0
4	A	903	STU	4	0
4	A	901	STU	3	0

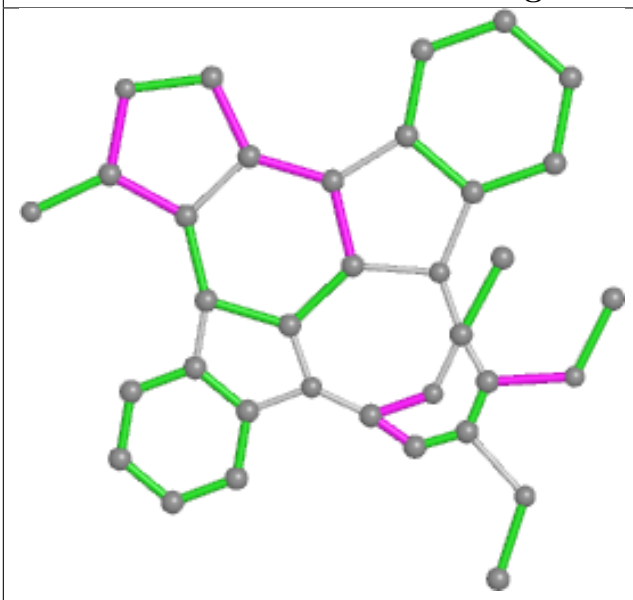
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

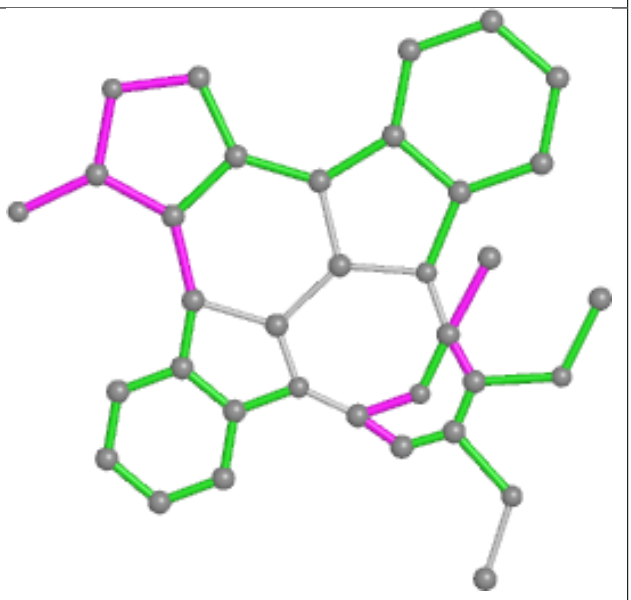
Ligand STU A 902



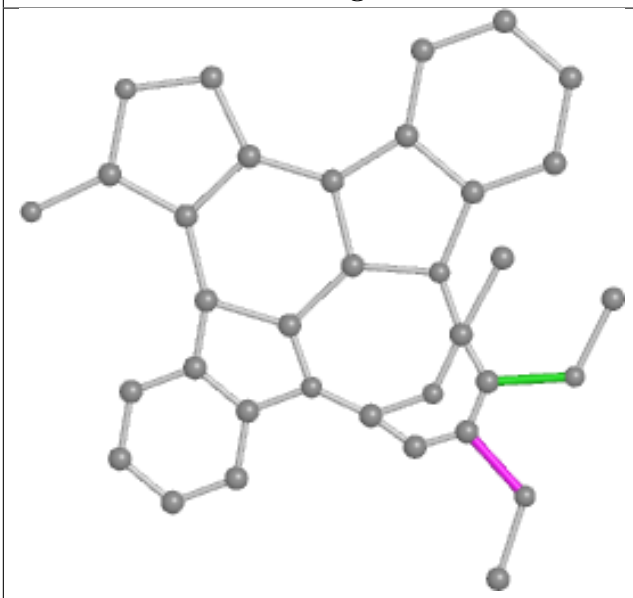
Ligand STU A 903



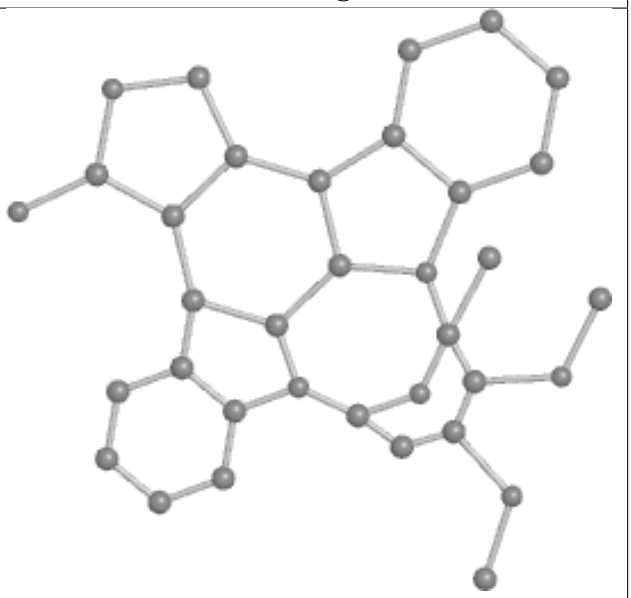
Bond lengths



Bond angles

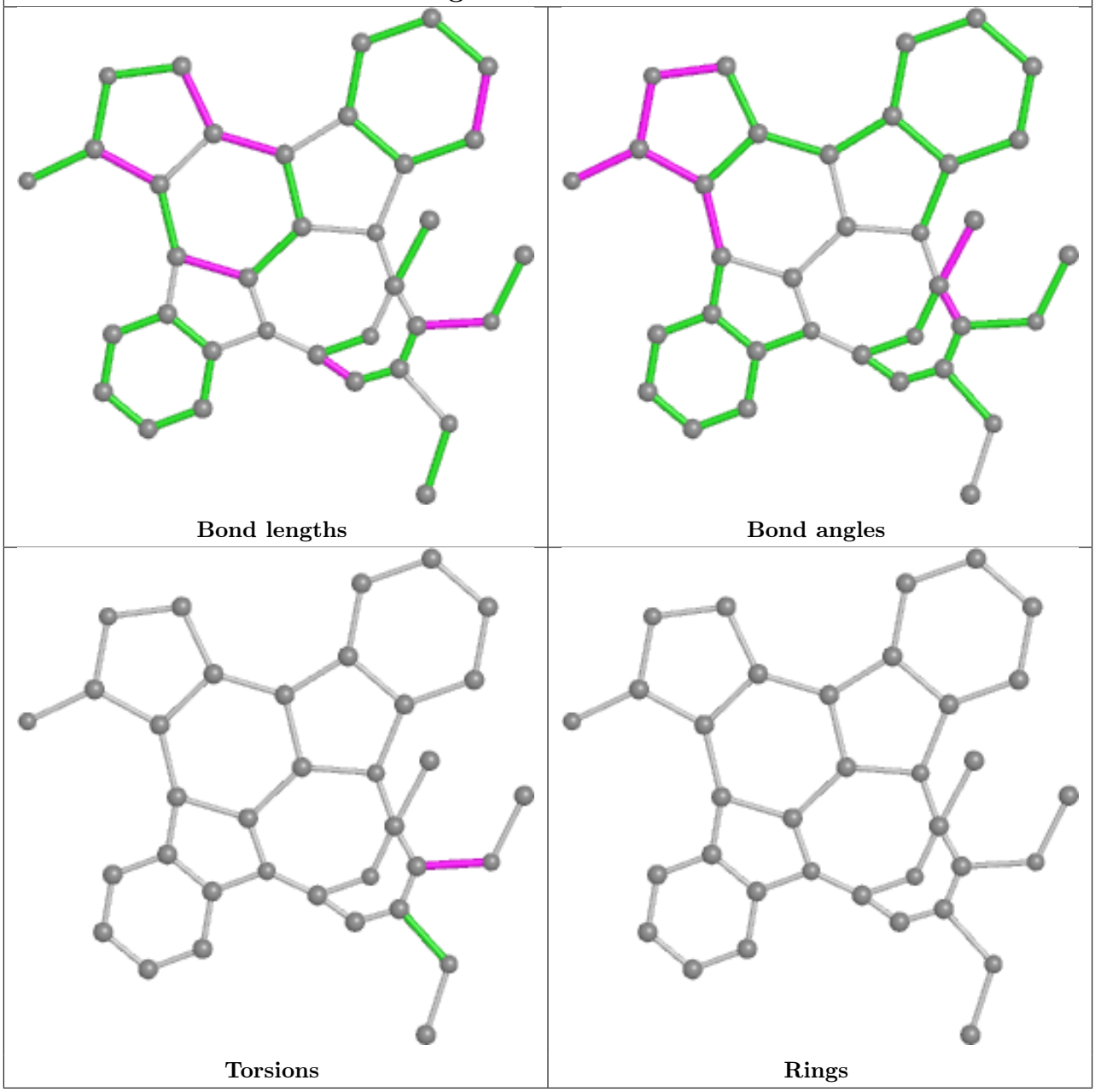


Torsions



Rings

Ligand STU A 901



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	A	352/377 (93%)	2.36	166 (47%) 0 0	35, 47, 61, 74	0
2	B	5/6 (83%)	0.90	0 100 100	42, 42, 45, 49	0
All	All	357/383 (93%)	2.34	166 (46%) 0 0	35, 46, 61, 74	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	LEU	10.4
1	A	489	GLN	9.2
1	A	468	ALA	8.8
1	A	533	THR	8.1
1	A	471	ALA	7.7
1	A	543	VAL	7.4
1	A	513	TYR	6.9
1	A	515	LEU	6.8
1	A	541	SER	6.7
1	A	530	LEU	6.5
1	A	473	LEU	6.3
1	A	532	SER	6.3
1	A	495	VAL	6.2
1	A	545	LEU	6.1
1	A	600	LEU	6.1
1	A	531	LEU	6.1
1	A	598	PRO	6.1
1	A	466	PRO	6.1
1	A	503	HIS	5.9
1	A	475	VAL	5.8
1	A	476	HIS	5.6
1	A	527	ILE	5.6
1	A	523	ILE	5.5
1	A	536	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	474	LEU	5.3
1	A	504	PHE	5.2
1	A	549	VAL	5.1
1	A	599	ASP	4.9
1	A	467	ARG	4.9
1	A	542	GLY	4.8
1	A	511	ASN	4.8
1	A	524	PRO	4.8
1	A	470	VAL	4.8
1	A	716	SER	4.8
1	A	763	ASN	4.6
1	A	482	VAL	4.6
1	A	544	VAL	4.5
1	A	479	ASP	4.5
1	A	501	PRO	4.5
1	A	537	LEU	4.5
1	A	454	PRO	4.5
1	A	455	LEU	4.5
1	A	449	PRO	4.4
1	A	534	GLN	4.4
1	A	506	ILE	4.3
1	A	719	LEU	4.3
1	A	764	LEU	4.3
1	A	521	PRO	4.3
1	A	485	SER	4.2
1	A	792	LEU	4.2
1	A	490	GLU	4.1
1	A	529	HIS	4.1
1	A	477	SER	4.1
1	A	505	ILE	4.1
1	A	526	LEU	4.1
1	A	514	ARG	4.0
1	A	691	VAL	4.0
1	A	769	THR	4.0
1	A	502	ARG	4.0
1	A	480	PHE	3.9
1	A	567	ILE	3.9
1	A	680	ILE	3.9
1	A	623[A]	ILE	3.9
1	A	478	GLY	3.8
1	A	546	HIS	3.8
1	A	630	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	571[A]	ASN	3.8
1	A	448	ILE	3.7
1	A	810	ILE	3.7
1	A	756	LEU	3.7
1	A	464	ALA	3.7
1	A	679	CYS	3.7
1	A	690	LEU	3.7
1	A	469	GLU	3.7
1	A	493	LEU	3.6
1	A	814	LEU	3.6
1	A	743	VAL	3.6
1	A	674	LEU	3.5
1	A	484	GLU	3.5
1	A	602	ALA	3.5
1	A	807	PHE	3.5
1	A	465	ILE	3.4
1	A	535	GLN	3.4
1	A	528	ASP	3.4
1	A	619	ILE	3.3
1	A	472	GLU	3.3
1	A	481	LEU	3.3
1	A	734	TYR	3.3
1	A	451	VAL	3.3
1	A	452	GLN	3.1
1	A	550	PRO	3.1
1	A	611	LEU	3.1
1	A	575	VAL	3.1
1	A	610	ILE	3.1
1	A	580	LEU	3.0
1	A	710	ASP	3.0
1	A	781	CYS	3.0
1	A	796	CYS	3.0
1	A	726	TRP	3.0
1	A	461	TYR	3.0
1	A	729	PRO	3.0
1	A	767	GLN	2.9
1	A	460	TRP	2.9
1	A	547	ARG	2.9
1	A	644	PHE	2.9
1	A	744	TRP	2.8
1	A	522	SER	2.8
1	A	697	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	686	ALA	2.7
1	A	773	VAL	2.7
1	A	447	MET	2.7
1	A	771	GLU	2.7
1	A	694	LYS	2.6
1	A	587	VAL	2.6
1	A	660	LEU	2.6
1	A	699[A]	ILE	2.6
1	A	762	PRO	2.6
1	A	789	VAL	2.6
1	A	648	LEU	2.6
1	A	620	VAL	2.6
1	A	483	ARG	2.5
1	A	655	LEU	2.5
1	A	804	ARG	2.5
1	A	463	GLY	2.5
1	A	678	CYS	2.5
1	A	639	VAL	2.5
1	A	627	THR	2.5
1	A	491	TYR	2.4
1	A	732	LEU	2.4
1	A	821	HIS	2.4
1	A	664	VAL	2.4
1	A	589	VAL	2.4
1	A	791	ARG	2.4
1	A	779	LEU	2.3
1	A	689	CYS	2.3
1	A	659	THR	2.3
1	A	525	LEU	2.3
1	A	622	LEU	2.3
1	A	751	TRP	2.3
1	A	576	PHE	2.2
1	A	634	ILE	2.2
1	A	739[A]	SER	2.2
1	A	456	HIS	2.2
1	A	684	LEU	2.2
1	A	582	ALA	2.2
1	A	709	ALA	2.2
1	A	722	VAL	2.2
1	A	647	PHE	2.2
1	A	733	ASN	2.2
1	A	453	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	2.2
1	A	746	PHE	2.1
1	A	608	ALA	2.1
1	A	702	PHE	2.1
1	A	662	GLN	2.1
1	A	450	GLU	2.1
1	A	805	PRO	2.1
1	A	797	TRP	2.1
1	A	638	LEU	2.1
1	A	760	PRO	2.1
1	A	784	LEU	2.1
1	A	605	LEU	2.0
1	A	793	MET	2.0
1	A	724	VAL	2.0
1	A	554	TRP	2.0
1	A	586	LEU	2.0

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	A	713	16/17	0.76	0.22	40,47,77,79	0

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, 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
4	STU	A	903	35/35	0.80	0.23	36,45,63,73	0

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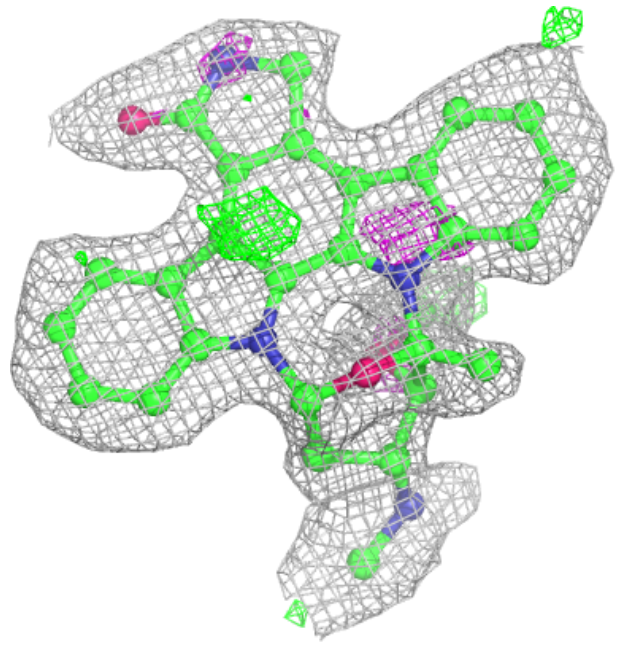
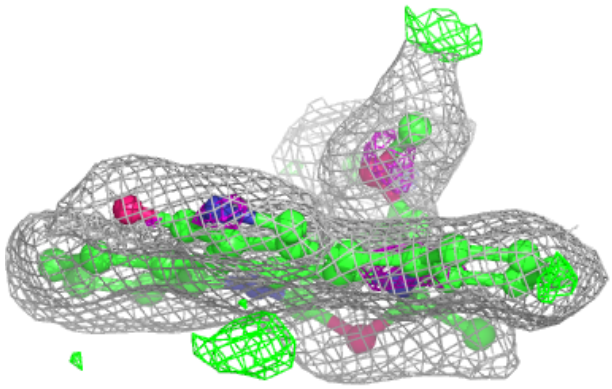
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	STU	A	902	35/35	0.86	0.20	33,43,50,61	0
4	STU	A	901	35/35	0.88	0.16	28,33,40,49	0
3	CL	A	905	1/1	0.97	0.12	47,47,47,47	0
3	CL	A	904	1/1	0.97	0.09	39,39,39,39	0

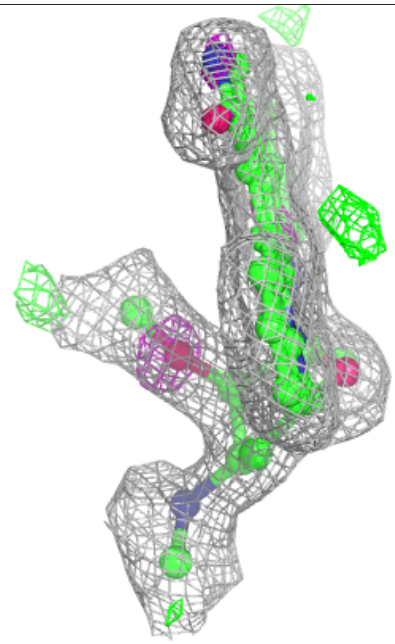
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

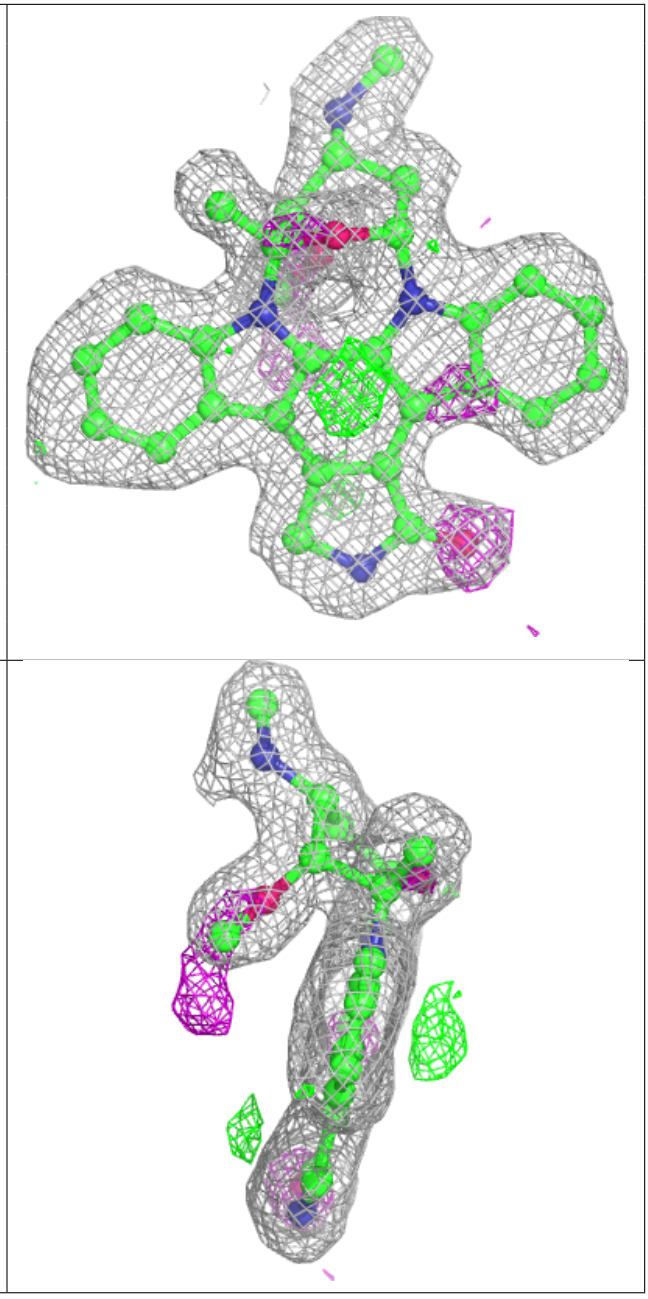






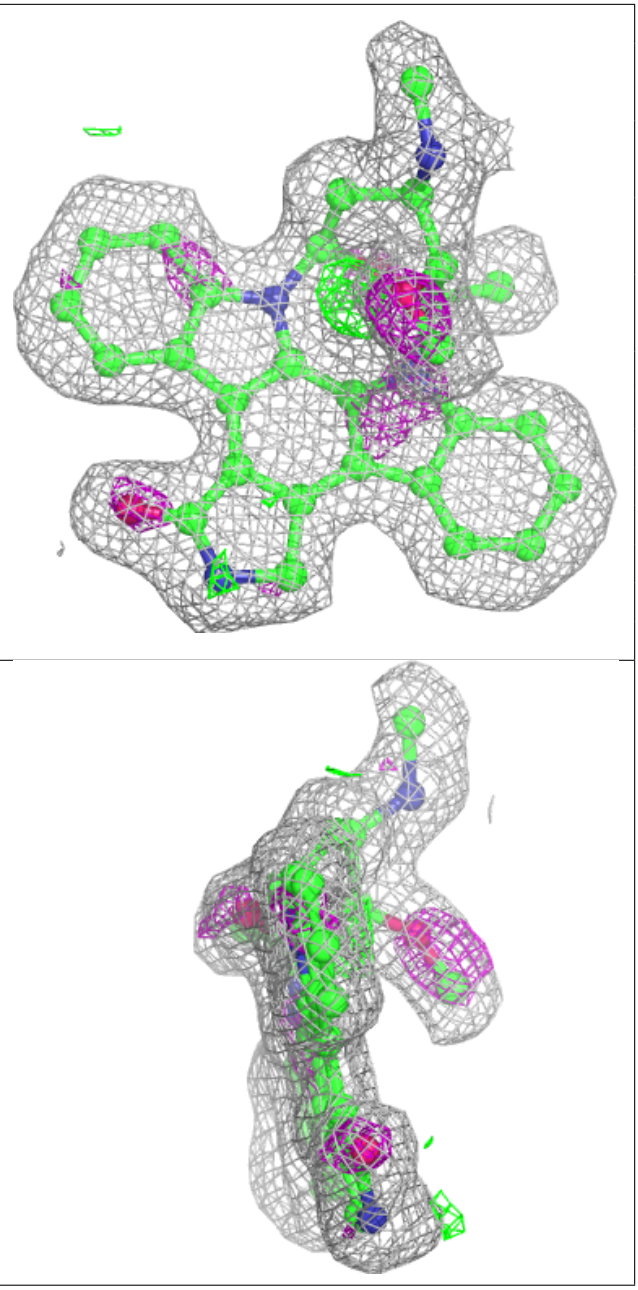
Electron density around STU A 902:

$2mF_o$-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 (i)

There are no such residues in this entry.