



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2020 – 06:07 PM EST

PDB ID : 6W8I
Title : Ternary complex structure - BTK cIAP compound 15
Authors : Calabrese, M.F.; Schiemer, J.S.
Deposited on : 2020-03-20
Resolution : 3.80 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.14.6
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) : 2.14.6

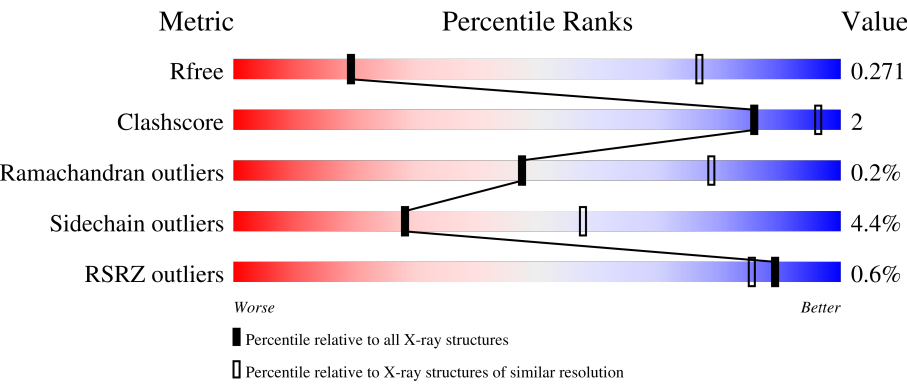
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 on 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	277	<div><div></div><div>82%9%8%</div></div>
1	B	277	<div><div>%</div><div>80%10%9%</div></div>
1	C	277	<div><div></div><div>87%7%5%</div></div>
2	D	99	<div><div></div><div>83%9%7%</div></div>
2	E	99	<div><div></div><div>87%7%6%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	99	<div><div></div><div>2%</div><div>85%</div><div>6% • 8%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8464 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 Tyrosine-protein kinase BTK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1970	1271	326	358	15			
1	B	251	Total	C	N	O	S	0	0	0
			2001	1287	332	364	18			
1	C	263	Total	C	N	O	S	0	0	0
			2068	1333	335	381	19			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	SER	-	expression tag	UNP Q06187
B	383	SER	-	expression tag	UNP Q06187
C	383	SER	-	expression tag	UNP Q06187

- Molecule 2 is a protein called Baculoviral IAP repeat-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	92	Total	C	N	O	S	0	0	0
			727	462	127	129	9			
2	E	93	Total	C	N	O	S	0	0	0
			745	475	126	135	9			
2	F	91	Total	C	N	O	S	0	0	0
			695	444	117	126	8			

There are 18 discrepancies between the modelled and reference sequences:

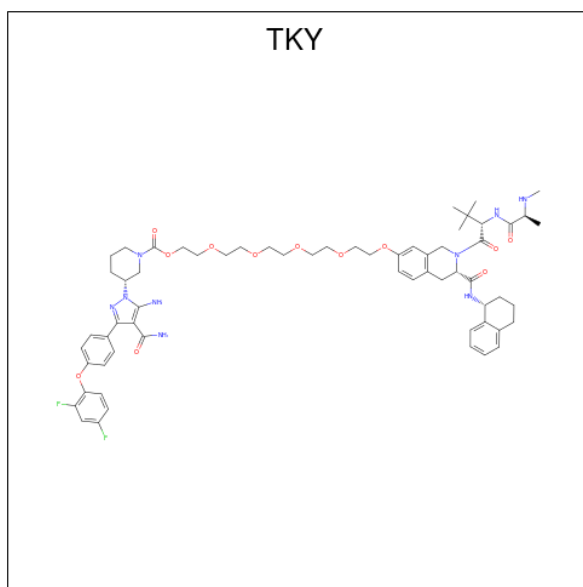
Chain	Residue	Modelled	Actual	Comment	Reference
D	254	GLY	-	expression tag	UNP Q13490
D	255	SER	-	expression tag	UNP Q13490
D	256	GLY	-	expression tag	UNP Q13490
D	257	PRO	-	expression tag	UNP Q13490
D	258	GLY	-	expression tag	UNP Q13490

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Chain	Residue	Modelled	Actual	Comment	Reference
D	259	SER	-	expression tag	UNP Q13490
E	254	GLY	-	expression tag	UNP Q13490
E	255	SER	-	expression tag	UNP Q13490
E	256	GLY	-	expression tag	UNP Q13490
E	257	PRO	-	expression tag	UNP Q13490
E	258	GLY	-	expression tag	UNP Q13490
E	259	SER	-	expression tag	UNP Q13490
F	254	GLY	-	expression tag	UNP Q13490
F	255	SER	-	expression tag	UNP Q13490
F	256	GLY	-	expression tag	UNP Q13490
F	257	PRO	-	expression tag	UNP Q13490
F	258	GLY	-	expression tag	UNP Q13490
F	259	SER	-	expression tag	UNP Q13490

- Molecule 3 is 14-{[(3S)-2-(N-methyl-L-alanyl-3-methyl-L-valyl)-3-{[(1R)-1,2,3,4-tetrahydro naphthalen-1-yl]carbamoyl}-1,2,3,4-tetrahydroisoquinolin-7-yl]oxy}-3,6,9,12-tetraoxatetra decan-1-yl (3R)-3-{5-amino-4-carbamoyl-3-[4-(2,4-difluorophenoxy)phenyl]-1H-pyrazol-1-yl]piperidine-1-carboxylate (three-letter code: TKY) (formula: C₆₂H₇₉F₂N₉O₁₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	F	N	O	0	0
			85	62	2	9	12		
3	D	1	Total	C	F	N	O	0	0
			85	62	2	9	12		
3	E	1	Total	C	F	N	O	0	0
			85	62	2	9	12		

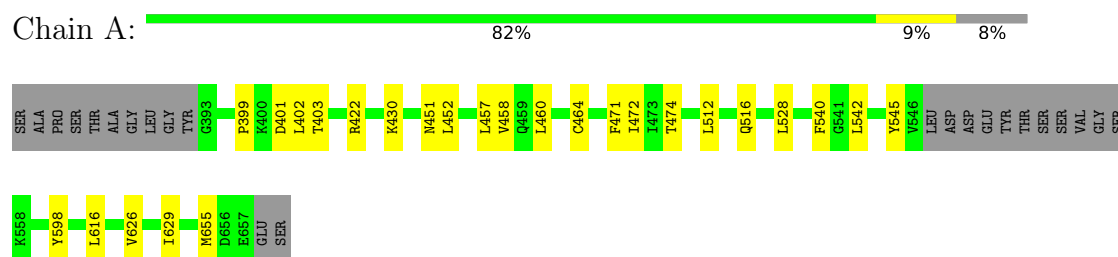
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total 1	Zn 1	0	0
4	F	1	Total 1	Zn 1	0	0
4	E	1	Total 1	Zn 1	0	0

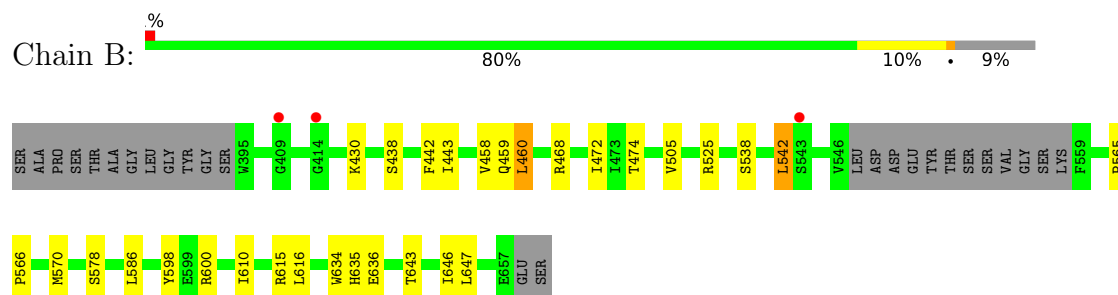
3 Residue-property plots [i](#)

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.

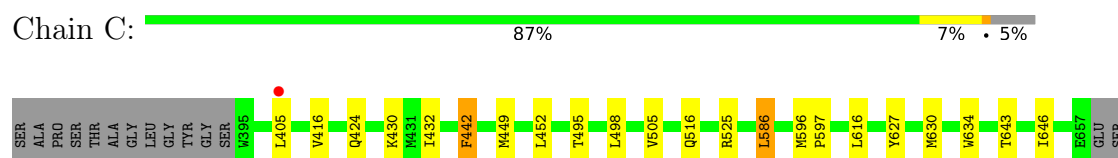
- Molecule 1: Tyrosine-protein kinase BTK



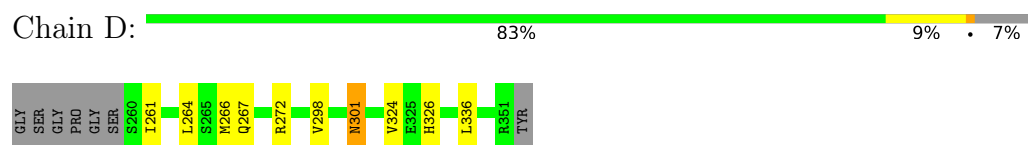
- Molecule 1: Tyrosine-protein kinase BTK



- Molecule 1: Tyrosine-protein kinase BTK



- Molecule 2: Baculoviral IAP repeat-containing protein 2

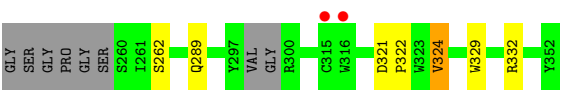
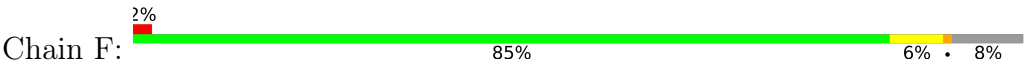


- Molecule 2: Baculoviral IAP repeat-containing protein 2





● Molecule 2: Baculoviral IAP repeat-containing protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.25Å 109.49Å 188.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.80 49.74 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.74-3.80) 99.9 (49.74-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.211 , 0.251 0.222 , 0.271	Depositor DCC
R_{free} test set	745 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8464	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: ZN, TKY

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	0.39	0/2018	0.59	0/2740
1	B	0.39	0/2048	0.58	0/2770
1	C	0.40	0/2118	0.59	0/2871
2	D	0.36	0/750	0.54	0/1017
2	E	0.37	0/769	0.54	0/1042
2	F	0.38	0/717	0.54	0/975
All	All	0.39	0/8420	0.58	0/11415

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	1970	0	1847	10	0
1	B	2001	0	1926	10	0
1	C	2068	0	1960	10	0
2	D	727	0	661	3	0
2	E	745	0	678	1	0
2	F	695	0	597	4	0
3	C	85	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	85	0	0	0	0
3	E	85	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	8464	0	7669	36	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 2.

All (36) 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:C:505:VAL:HG11	1:C:586:LEU:HD21	1.85	0.58
1:C:416:VAL:HG22	1:C:430:LYS:HG3	1.85	0.57
1:C:432:ILE:HG21	1:C:442:PHE:HE2	1.70	0.56
1:B:643:THR:H	1:B:646:ILE:HD12	1.69	0.56
1:A:399:PRO:HA	1:A:402:LEU:HD12	1.90	0.55
1:C:405:LEU:HB3	2:F:329:TRP:CZ3	2.43	0.54
1:A:460:LEU:HA	1:A:474:THR:HG22	1.88	0.53
2:D:261:ILE:HD13	2:D:267:GLN:HE21	1.73	0.53
1:C:495:THR:HA	1:C:498:LEU:HD12	1.91	0.52
1:C:643:THR:H	1:C:646:ILE:HD12	1.75	0.51
1:B:615:ARG:HD2	1:B:634:TRP:HB3	1.93	0.50
1:A:626:VAL:HA	1:A:629:ILE:HD12	1.93	0.49
2:D:326:HIS:HB3	2:D:336:LEU:HD13	1.97	0.46
1:A:458:VAL:HG21	1:A:528:LEU:HD12	1.98	0.46
2:E:297:TYR:HA	2:E:304:VAL:HG12	1.98	0.45
1:A:542:LEU:HA	1:A:545:TYR:HD2	1.81	0.45
1:B:566:PRO:HG3	1:B:610:ILE:HG22	1.97	0.45
1:B:598:TYR:CZ	1:B:616:LEU:HG	2.52	0.45
1:A:430:LYS:HB3	1:A:472:ILE:HB	1.97	0.45
2:F:321:ASP:HB3	2:F:324:VAL:HB	1.99	0.45
1:C:449:MET:HA	1:C:452:LEU:HD12	1.98	0.44
1:A:542:LEU:HA	1:A:545:TYR:CD2	2.53	0.43
1:C:627:TYR:HA	1:C:630:MET:HG2	2.00	0.43
1:C:424:GLN:HB2	2:F:332:ARG:HD3	2.00	0.43
1:B:430:LYS:HB3	1:B:472:ILE:HB	2.00	0.43
1:A:464:CYS:HB2	1:A:471:PHE:HB2	2.00	0.43
1:A:598:TYR:CZ	1:A:616:LEU:HG	2.54	0.42
1:B:542:LEU:HD22	1:B:542:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:289:GLN:HB3	2:F:322:PRO:HG2	2.02	0.42
1:A:457:LEU:HD11	1:A:512:LEU:HD21	2.01	0.42
1:B:505:VAL:HG11	1:B:586:LEU:HD21	2.03	0.41
1:B:565:PRO:HG3	1:B:578:SER:HA	2.02	0.41
1:B:458:VAL:HG21	1:B:538:SER:HB3	2.03	0.40
1:B:460:LEU:HA	1:B:474:THR:HG22	2.03	0.40
2:D:266:MET:HB3	2:D:272:ARG:HG2	2.02	0.40
1:C:597:PRO:HB3	1:C:616:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

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	250/277 (90%)	235 (94%)	15 (6%)	0	100	100
1	B	247/277 (89%)	234 (95%)	12 (5%)	1 (0%)	34	70
1	C	261/277 (94%)	247 (95%)	14 (5%)	0	100	100
2	D	90/99 (91%)	86 (96%)	3 (3%)	1 (1%)	14	51
2	E	91/99 (92%)	87 (96%)	4 (4%)	0	100	100
2	F	87/99 (88%)	81 (93%)	6 (7%)	0	100	100
All	All	1026/1128 (91%)	970 (94%)	54 (5%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	438	SER
2	D	301	ASN

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	199/247 (81%)	191 (96%)	8 (4%)	31	59
1	B	211/247 (85%)	199 (94%)	12 (6%)	20	52
1	C	215/247 (87%)	209 (97%)	6 (3%)	43	68
2	D	75/84 (89%)	71 (95%)	4 (5%)	22	54
2	E	78/84 (93%)	73 (94%)	5 (6%)	17	48
2	F	67/84 (80%)	65 (97%)	2 (3%)	41	66
All	All	845/993 (85%)	808 (96%)	37 (4%)	28	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	401	ASP
1	A	403	THR
1	A	422	ARG
1	A	451	ASN
1	A	452	LEU
1	A	516	GLN
1	A	540	PHE
1	A	655	MET
1	B	442	PHE
1	B	443	ILE
1	B	459	GLN
1	B	460	LEU
1	B	468	ARG
1	B	525	ARG
1	B	542	LEU
1	B	570	MET
1	B	600	ARG
1	B	635	HIS
1	B	636	GLU
1	B	647	LEU
1	C	442	PHE
1	C	516	GLN

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Mol	Chain	Res	Type
1	C	525	ARG
1	C	586	LEU
1	C	596	MET
1	C	634	TRP
2	D	264	LEU
2	D	298	VAL
2	D	301	ASN
2	D	324	VAL
2	E	261	ILE
2	E	330	PHE
2	E	334	GLU
2	E	340	LYS
2	E	352	TYR
2	F	262	SER
2	F	324	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	267	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](#)

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](#)

Of 6 ligands modelled in this entry, 3 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
3	TKY	E	502	-	91,92,92	0.51	2 (2%)	115,128,128	0.72	3 (2%)
3	TKY	D	502	-	91,92,92	0.52	3 (3%)	115,128,128	0.74	3 (2%)
3	TKY	C	701	-	91,92,92	0.53	2 (2%)	115,128,128	0.78	4 (3%)

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	TKY	E	502	-	-	14/63/103/103	0/8/8/8
3	TKY	D	502	-	-	19/63/103/103	0/8/8/8
3	TKY	C	701	-	-	16/63/103/103	0/8/8/8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	TKY	C59-N60	-2.76	1.33	1.35
3	E	502	TKY	C59-N60	-2.75	1.33	1.35
3	C	701	TKY	C58-C59	2.75	1.44	1.41
3	D	502	TKY	C59-N60	-2.62	1.33	1.35
3	D	502	TKY	C58-C59	2.54	1.44	1.41
3	E	502	TKY	C58-C59	2.45	1.44	1.41
3	D	502	TKY	C58-C76	-2.14	1.47	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	502	TKY	C23-C22-C27	3.91	116.59	111.34
3	C	701	TKY	C6-N5-C3	3.76	129.83	122.05
3	D	502	TKY	C6-N5-C3	3.69	129.70	122.05
3	C	701	TKY	C23-C22-C27	3.17	115.60	111.34
3	D	502	TKY	C23-C22-C27	2.89	115.22	111.34
3	E	502	TKY	C68-O67-C64	2.51	124.27	118.00
3	C	701	TKY	C68-O67-C64	2.45	124.11	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	TKY	C68-O67-C64	2.41	124.01	118.00
3	E	502	TKY	C6-N5-C3	2.40	127.02	122.05
3	C	701	TKY	C59-C58-C76	2.08	131.13	127.08

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	502	TKY	N60-C59-C61-C62
3	E	502	TKY	N60-C59-C61-C66
3	D	502	TKY	C1-C2-N84-C85
3	D	502	TKY	N60-C59-C61-C62
3	D	502	TKY	N60-C59-C61-C66
3	C	701	TKY	N60-C59-C61-C62
3	C	701	TKY	N60-C59-C61-C66
3	C	701	TKY	O35-C36-C37-O38
3	E	502	TKY	O38-C39-C40-O41
3	D	502	TKY	N5-C6-C80-C83
3	D	502	TKY	N5-C6-C80-C82
3	D	502	TKY	O44-C45-C46-O47
3	C	701	TKY	O41-C42-C43-O44
3	D	502	TKY	N5-C6-C80-C81
3	E	502	TKY	C1-C2-N84-C85
3	C	701	TKY	C1-C2-N84-C85
3	C	701	TKY	N5-C6-C80-C83
3	D	502	TKY	C34-C33-O32-C13
3	C	701	TKY	C43-C42-O41-C40
3	C	701	TKY	N5-C6-C80-C82
3	E	502	TKY	C42-C43-O44-C45
3	C	701	TKY	C36-C37-O38-C39
3	E	502	TKY	C36-C37-O38-C39
3	E	502	TKY	C37-C36-O35-C34
3	E	502	TKY	C40-C39-O38-C37
3	C	701	TKY	C42-C43-O44-C45
3	D	502	TKY	C46-C45-O44-C43
3	C	701	TKY	C39-C40-O41-C42
3	C	701	TKY	N5-C6-C80-C81
3	D	502	TKY	C7-C6-C80-C81
3	D	502	TKY	C7-C6-C80-C82
3	E	502	TKY	C39-C40-O41-C42
3	C	701	TKY	C46-C45-O44-C43
3	D	502	TKY	C40-C39-O38-C37

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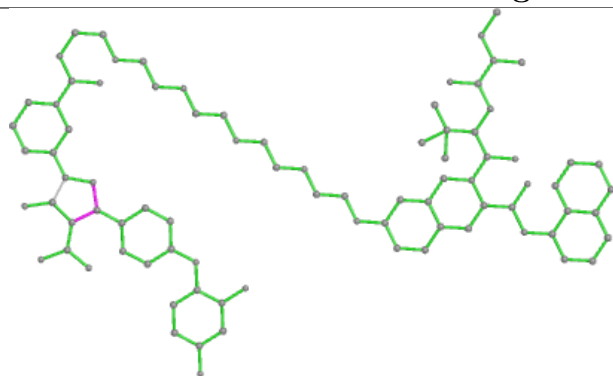
Mol	Chain	Res	Type	Atoms
3	E	502	TKY	C34-C33-O32-C13
3	E	502	TKY	C3-C2-N84-C85
3	D	502	TKY	C3-C2-N84-C85
3	C	701	TKY	C3-C2-N84-C85
3	D	502	TKY	C33-C34-O35-C36
3	D	502	TKY	C36-C37-O38-C39
3	E	502	TKY	C43-C42-O41-C40
3	D	502	TKY	C43-C42-O41-C40
3	D	502	TKY	O41-C42-C43-O44
3	D	502	TKY	C39-C40-O41-C42
3	D	502	TKY	C7-C6-C80-C83
3	E	502	TKY	O49-C48-N50-C55
3	C	701	TKY	C34-C33-O32-C13
3	C	701	TKY	C40-C39-O38-C37
3	E	502	TKY	O35-C36-C37-O38

There are no ring outliers.

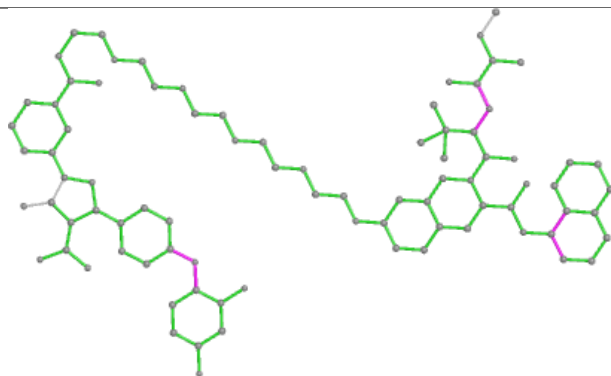
No monomer is involved in short contacts.

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.

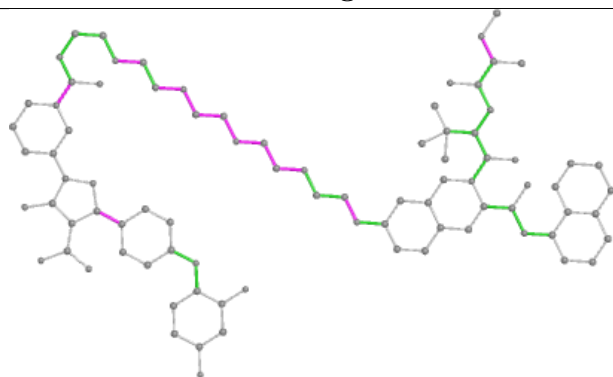
Ligand TKY E 502



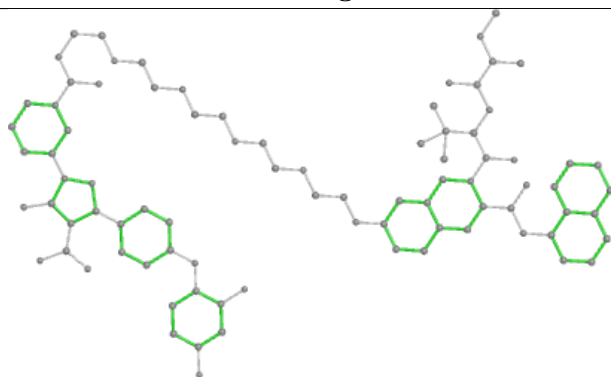
Bond lengths



Bond angles

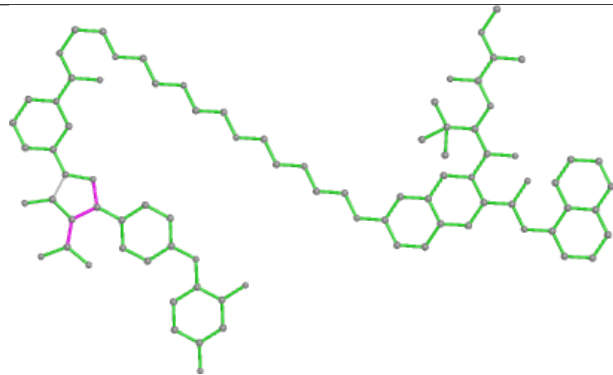


Torsions

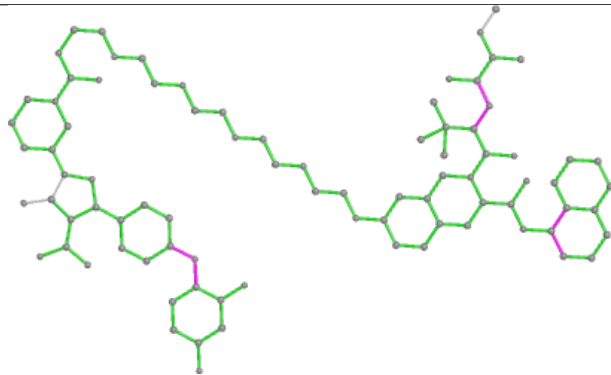


Rings

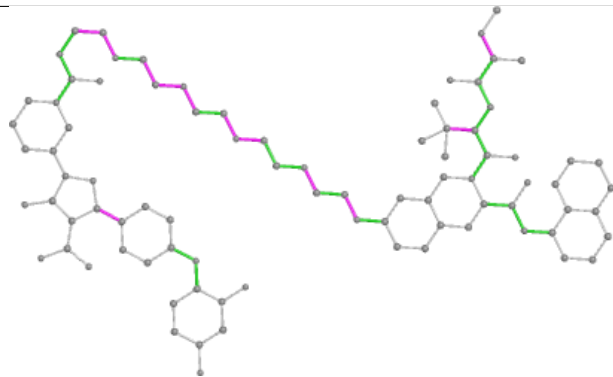
Ligand TKY D 502



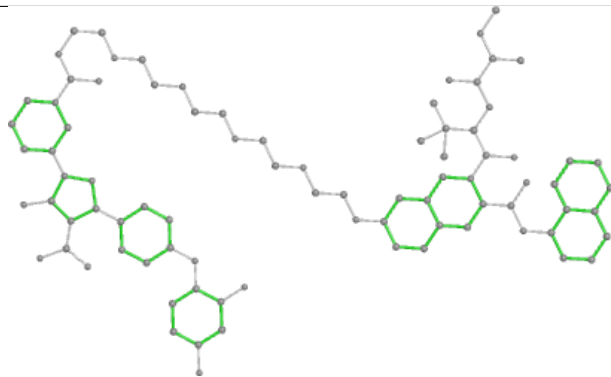
Bond lengths



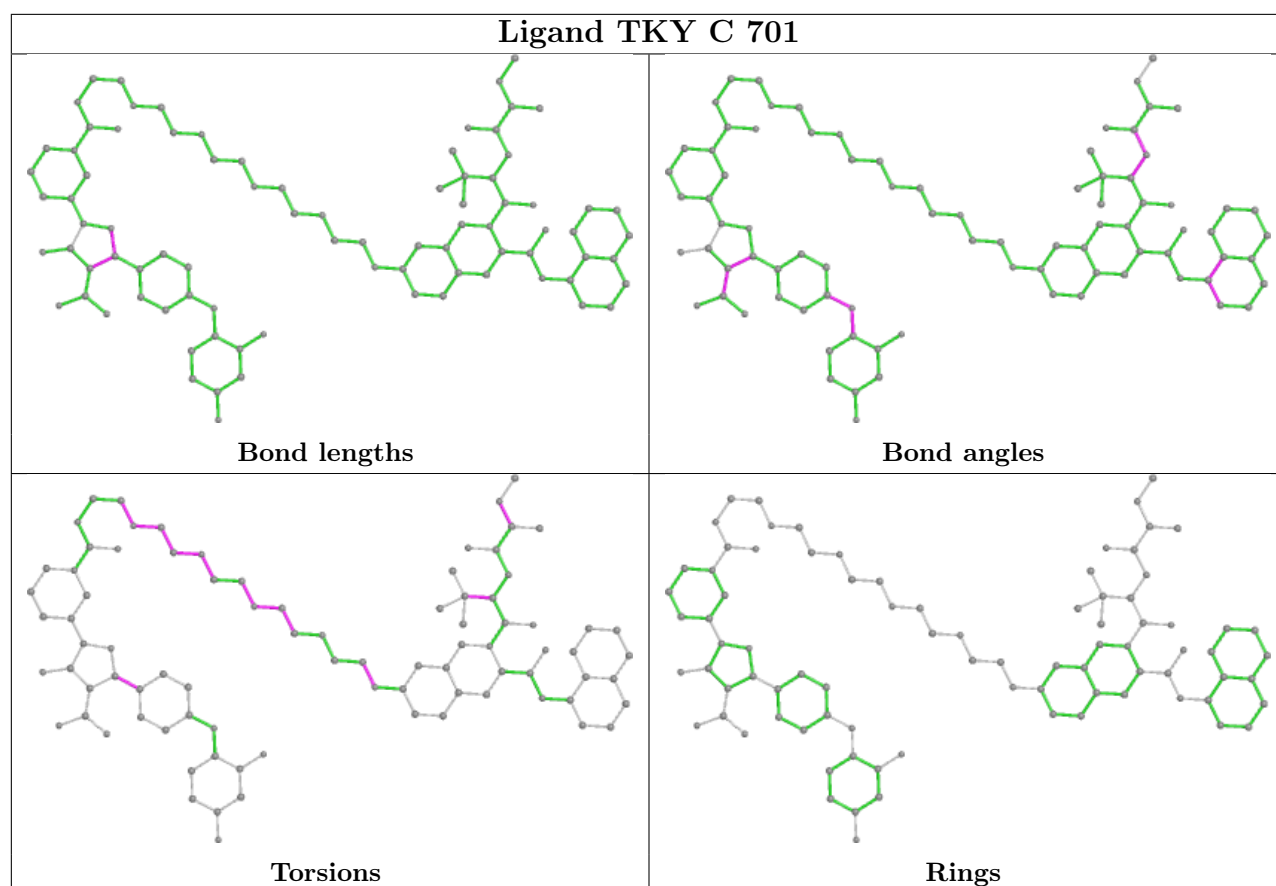
Bond angles



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 [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	254/277 (91%)	-0.08	0 100 100	22, 45, 89, 97	0
1	B	251/277 (90%)	0.01	3 (1%) 79 72	29, 47, 75, 100	0
1	C	263/277 (94%)	-0.11	1 (0%) 92 89	26, 52, 82, 93	0
2	D	92/99 (92%)	-0.17	0 100 100	27, 42, 58, 65	0
2	E	93/99 (93%)	-0.09	0 100 100	22, 42, 61, 72	0
2	F	91/99 (91%)	0.54	2 (2%) 62 54	34, 70, 140, 168	0
All	All	1044/1128 (92%)	-0.02	6 (0%) 89 85	22, 48, 85, 168	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	543	SER	4.2
1	B	414	GLY	2.5
2	F	315	CYS	2.4
1	C	405	LEU	2.4
1	B	409	GLY	2.0
2	F	316	TRP	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](#)

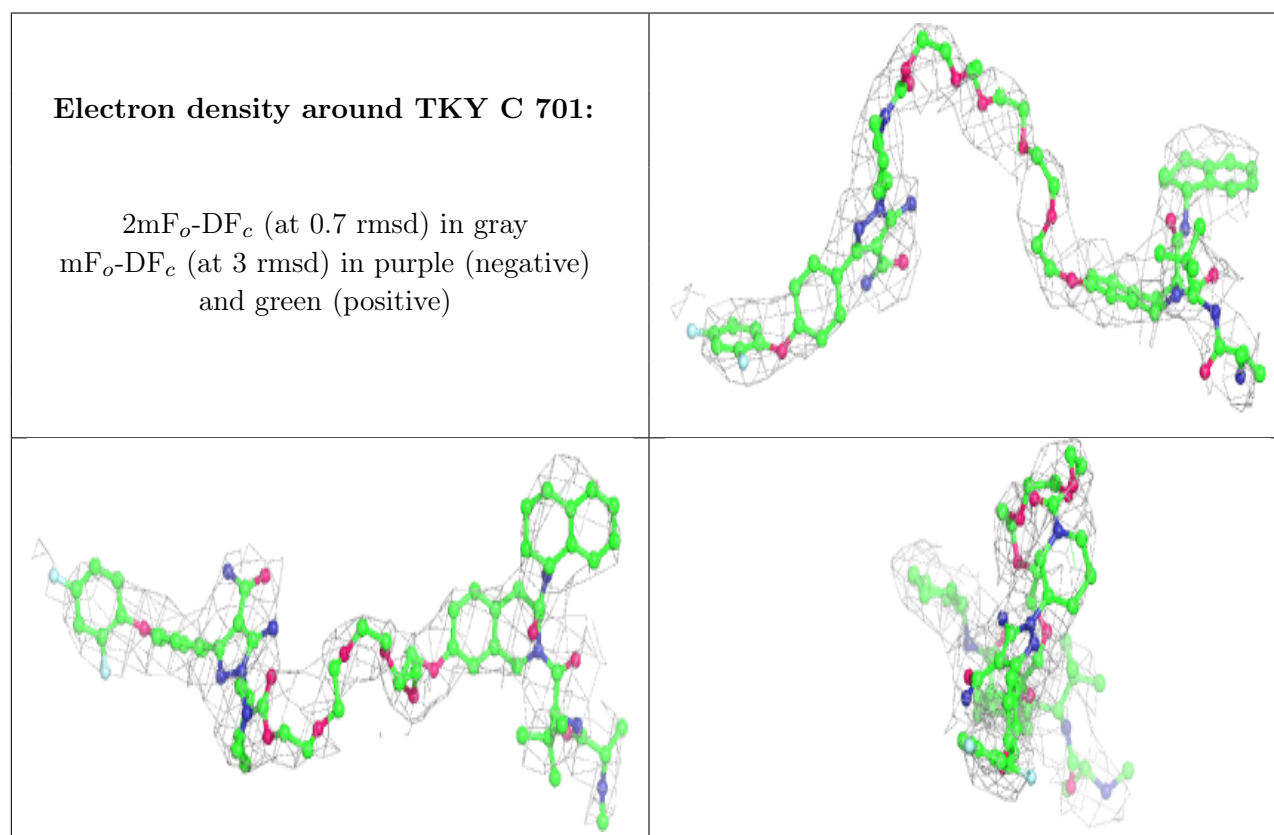
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

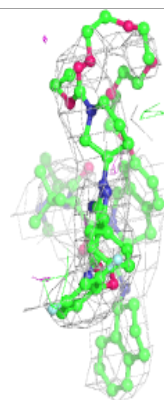
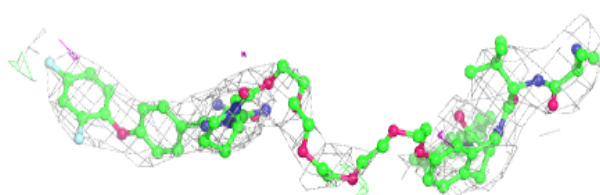
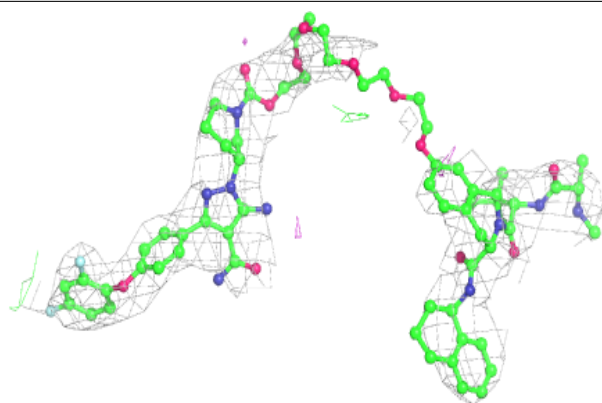
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TKY	C	701	85/85	0.88	0.44	40,58,78,80	0
3	TKY	E	502	85/85	0.90	0.38	33,47,83,84	0
3	TKY	D	502	85/85	0.91	0.37	31,43,71,76	0
4	ZN	F	501	1/1	0.98	0.09	60,60,60,60	0
4	ZN	E	501	1/1	0.99	0.12	33,33,33,33	0
4	ZN	D	501	1/1	1.00	0.14	28,28,28,28	0

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.

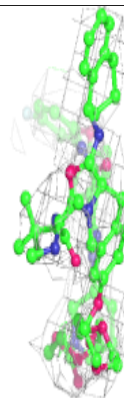
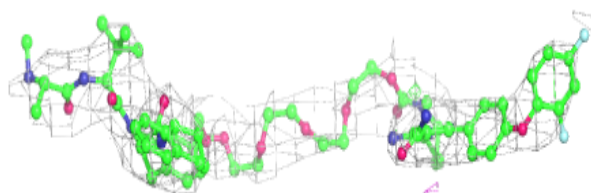
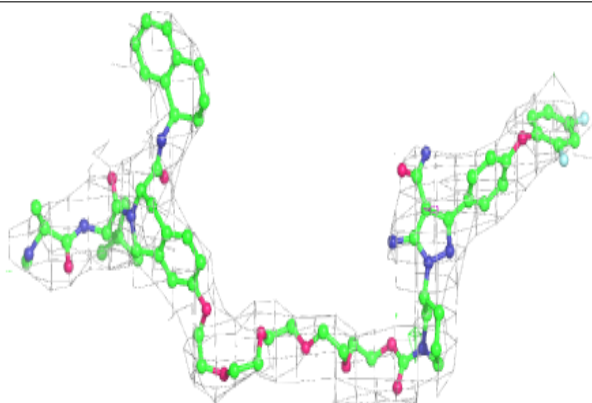


Electron density around TKY E 502:

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

**Electron density around TKY D 502:**

$2mF_o-DF_c$ (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.