



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2023 – 10:09 AM JST

PDB ID : 7YAW
Title : Crystal structure of ZAK in complex with compound YH-180
Authors : Kong, L.L.; Yun, C.H.
Deposited on : 2022-06-28
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.34
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) : 2.34

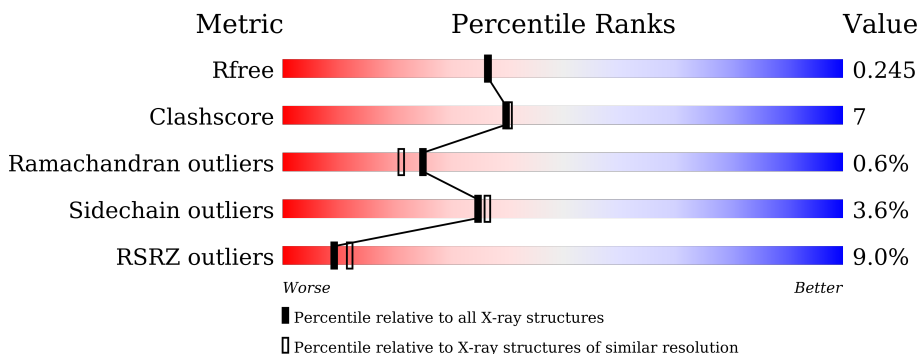
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	310	 7% 79% 13% • 6%
1	B	310	 8% 78% 14% • 6%
1	C	310	 9% 82% 10% • 6%
1	D	310	 10% 80% 13% • 6%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9900 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.

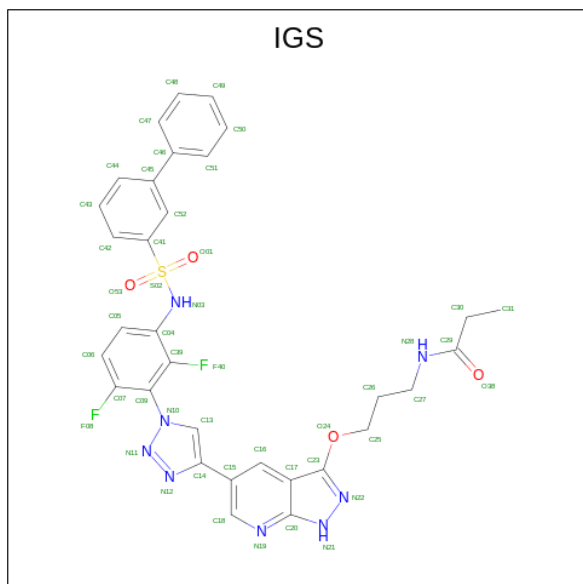
- Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase MLT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	291	2327	1491	389	432	15	0	1	0
1	A	291	2327	1491	389	432	15	0	1	0
1	B	291	2327	1491	389	432	15	0	1	0
1	C	291	2327	1491	389	432	15	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP Q9NYL2
D	1	ALA	-	expression tag	UNP Q9NYL2
D	2	MET	-	expression tag	UNP Q9NYL2
D	3	GLY	-	expression tag	UNP Q9NYL2
D	4	SER	-	expression tag	UNP Q9NYL2
A	0	GLY	-	expression tag	UNP Q9NYL2
A	1	ALA	-	expression tag	UNP Q9NYL2
A	2	MET	-	expression tag	UNP Q9NYL2
A	3	GLY	-	expression tag	UNP Q9NYL2
A	4	SER	-	expression tag	UNP Q9NYL2
B	0	GLY	-	expression tag	UNP Q9NYL2
B	1	ALA	-	expression tag	UNP Q9NYL2
B	2	MET	-	expression tag	UNP Q9NYL2
B	3	GLY	-	expression tag	UNP Q9NYL2
B	4	SER	-	expression tag	UNP Q9NYL2
C	0	GLY	-	expression tag	UNP Q9NYL2
C	1	ALA	-	expression tag	UNP Q9NYL2
C	2	MET	-	expression tag	UNP Q9NYL2
C	3	GLY	-	expression tag	UNP Q9NYL2
C	4	SER	-	expression tag	UNP Q9NYL2

- Molecule 2 is {N}-[3-[[5-[1-[2,6-bis(fluoranyl)-3-[(3-phenylphenyl)sulfonylamino]phenyl]-1,2,3-triazol-4-yl]-1 {H}-pyrazolo[3,4-b]pyridin-3-yl]oxy]propyl]propanamide (three-letter code: IGS) (formula: C₃₂H₂₈F₂N₈O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
2	D	1	Total	C	F	N	O	S	0	0
			47	32	2	8	4	1		
2	A	1	Total	C	F	N	O	S	0	0
			47	32	2	8	4	1		
2	B	1	Total	C	F	N	O	S	0	0
			47	32	2	8	4	1		
2	C	1	Total	C	F	N	O	S	0	0
			47	32	2	8	4	1		

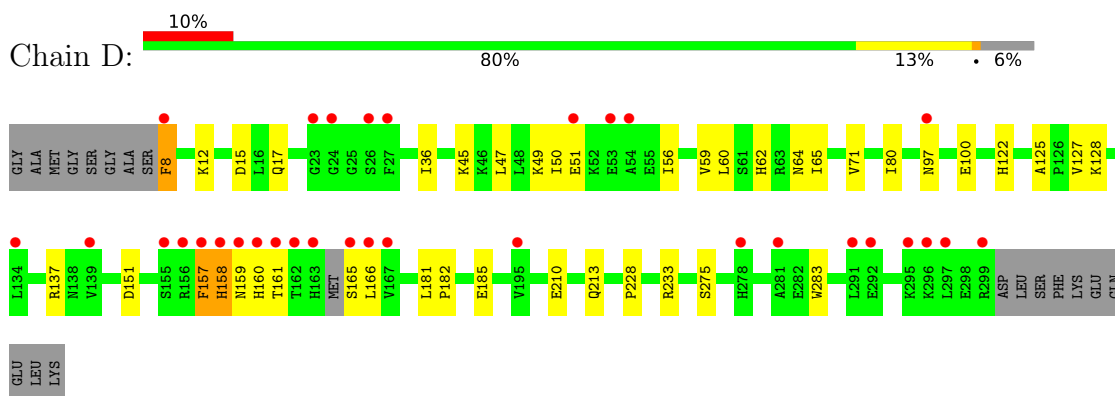
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	74	Total	O	0	0
			74	74		
3	A	124	Total	O	0	0
			124	124		
3	B	105	Total	O	0	0
			105	105		
3	C	101	Total	O	0	0
			101	101		

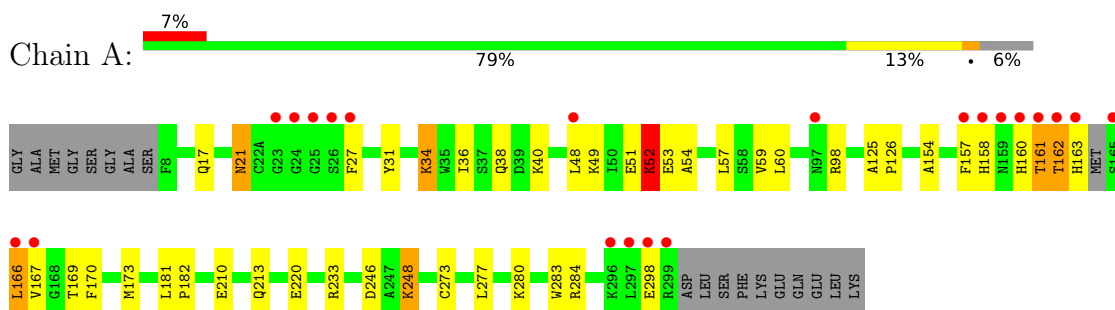
3 Residue-property plots [i](#)

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.

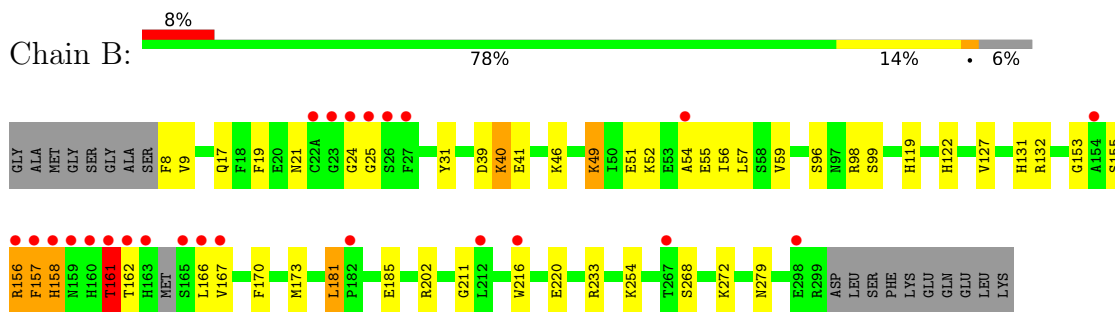
- Molecule 1: Mitogen-activated protein kinase kinase kinase MLT



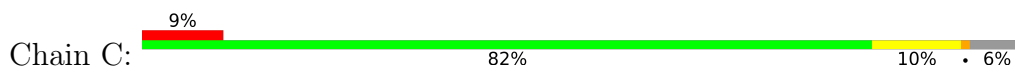
- Molecule 1: Mitogen-activated protein kinase kinase kinase MLT

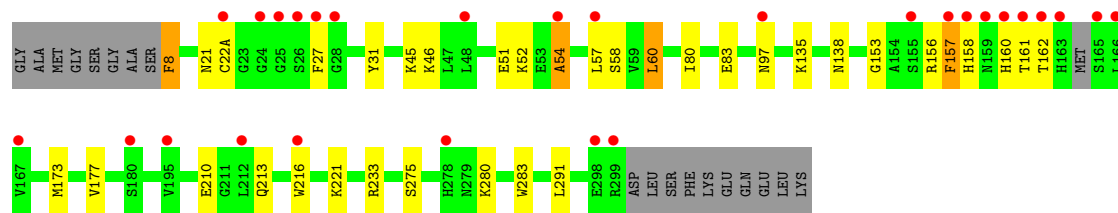


- Molecule 1: Mitogen-activated protein kinase kinase kinase MLT



- Molecule 1: Mitogen-activated protein kinase kinase kinase MLT





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.67Å 142.77Å 179.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.69 – 2.10 31.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.3 (31.69-2.10) 95.3 (31.69-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.207 , 0.243 0.214 , 0.245	Depositor DCC
R_{free} test set	4203 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9900	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.84% 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: IGS

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	0.45	0/2381	0.62	1/3222 (0.0%)
1	B	0.45	0/2381	0.64	0/3222
1	C	0.44	0/2380	0.64	2/3219 (0.1%)
1	D	0.42	0/2381	0.59	0/3222
All	All	0.44	0/9523	0.62	3/12885 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	PHE	CB-CG-CD1	5.91	124.94	120.80
1	C	157	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	A	52	LYS	CD-CE-NZ	-5.43	99.22	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	GLU	Peptide
1	B	17	GLN	Peptide
1	C	58[A]	SER	Mainchain
1	C	58[B]	SER	Mainchain

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	2327	0	2280	35	3
1	B	2327	0	2280	46	0
1	C	2327	0	2279	33	0
1	D	2327	0	2280	24	3
2	A	47	0	0	0	0
2	B	47	0	0	2	0
2	C	47	0	0	3	0
2	D	47	0	0	1	0
3	A	124	0	0	4	0
3	B	105	0	0	1	0
3	C	101	0	0	0	0
3	D	74	0	0	2	0
All	All	9900	0	9119	136	3

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 7.

All (136) 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:284:ARG:CD	3:A:501:HOH:O	2.16	0.92
1:A:48:LEU:HB3	1:A:160:HIS:HD2	1.33	0.91
1:A:284:ARG:HD3	3:A:501:HOH:O	1.72	0.86
1:C:57:LEU:HD11	1:C:153:GLY:HA3	1.59	0.85
1:A:210:GLU:HB2	1:A:213:GLN:HG3	1.62	0.82
1:B:57:LEU:HG	1:B:157:PHE:CZ	2.15	0.82
1:D:97:ASN:O	1:D:100:GLU:HG3	1.83	0.76
1:A:284:ARG:NE	3:A:501:HOH:O	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLN:HG3	1:A:36:ILE:HD11	1.72	0.71
1:A:48:LEU:HB3	1:A:160:HIS:CD2	2.22	0.70
1:B:57:LEU:H	1:B:157:PHE:HZ	1.41	0.68
1:A:59:VAL:HG12	1:A:126:PRO:HG2	1.75	0.68
1:A:34:LYS:NZ	1:B:39:ASP:OD2	2.26	0.67
1:A:213:GLN:HB3	1:A:298:GLU:OE2	1.95	0.66
1:B:9:VAL:HG12	3:B:557:HOH:O	1.95	0.65
1:B:57:LEU:HD11	1:B:153:GLY:HA3	1.82	0.61
1:D:50:ILE:HA	1:D:157:PHE:HZ	1.66	0.61
1:B:54:ALA:HA	1:B:157:PHE:CD1	2.36	0.61
1:C:31:TYR:HE1	1:C:46:LYS:HG3	1.66	0.60
1:C:51:GLU:O	1:C:54:ALA:HB3	2.02	0.60
1:B:40:LYS:HD3	1:B:41:GLU:O	2.02	0.59
1:A:161:THR:O	1:A:163:HIS:N	2.36	0.59
1:D:45:LYS:NZ	1:D:151:ASP:OD1	2.36	0.59
1:B:54:ALA:HA	1:B:157:PHE:CG	2.37	0.59
1:B:57:LEU:HG	1:B:157:PHE:CE1	2.37	0.59
1:B:153:GLY:O	1:B:157:PHE:HB2	2.02	0.58
1:D:47:LEU:HD12	1:D:50:ILE:HD13	1.85	0.58
1:D:47:LEU:HD11	1:D:80:ILE:CD1	2.34	0.58
1:B:49:LYS:HZ2	1:B:51:GLU:HG2	1.68	0.57
1:C:158:HIS:NE2	2:C:401:IGS:O53	2.37	0.57
1:D:60:LEU:HD22	1:D:125:ALA:HB1	1.87	0.56
1:C:173:MET:HE3	1:C:177:VAL:HG12	1.88	0.56
1:C:57:LEU:H	1:C:157:PHE:HZ	1.54	0.56
1:A:59:VAL:CG1	1:A:126:PRO:HG2	2.35	0.56
1:D:45:LYS:HE3	2:D:401:IGS:C04	2.35	0.55
1:D:62:HIS:HB3	1:D:65:ILE:HD13	1.87	0.55
1:D:122:HIS:CE1	1:D:185:GLU:HB2	2.41	0.55
1:A:213:GLN:HE21	1:A:298:GLU:CD	2.10	0.55
1:A:38:GLN:HB3	1:A:40:LYS:HD2	1.87	0.55
1:A:17:GLN:OE1	1:C:8:PHE:HB2	2.07	0.55
1:C:54:ALA:HA	1:C:157:PHE:CE2	2.42	0.55
1:B:216:TRP:CD1	1:B:220:GLU:HG3	2.42	0.54
1:C:153:GLY:O	1:C:157:PHE:HB2	2.07	0.54
1:A:49:LYS:H	1:A:160:HIS:CD2	2.25	0.54
1:A:280:LYS:HA	1:A:283:TRP:CE2	2.43	0.54
1:C:21:ASN:HB2	1:C:31:TYR:CE2	2.44	0.53
1:A:170:PHE:HA	1:A:173:MET:HE3	1.90	0.53
1:A:162:THR:HB	1:A:163:HIS:CD2	2.44	0.53
1:B:156:ARG:HD3	1:B:157:PHE:HD1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ALA:HA	1:C:157:PHE:CD2	2.45	0.52
1:A:57:LEU:HA	1:A:60:LEU:HD23	1.92	0.51
1:C:216:TRP:HH2	1:C:221:LYS:HZ3	1.57	0.51
1:B:96:SER:OG	1:B:98:ARG:HG2	2.09	0.51
1:A:169:THR:HG23	3:A:508:HOH:O	2.10	0.51
1:A:27:PHE:CZ	1:A:48:LEU:HD13	2.46	0.51
1:C:54:ALA:HA	1:C:157:PHE:CZ	2.45	0.51
1:B:21:ASN:HB2	1:B:31:TYR:CD2	2.46	0.51
1:A:158:HIS:O	1:A:158:HIS:ND1	2.45	0.50
1:D:137:ARG:HG3	3:D:523:HOH:O	2.12	0.50
1:C:173:MET:CE	1:C:177:VAL:HG12	2.41	0.50
1:B:40:LYS:HD3	1:B:41:GLU:N	2.26	0.50
1:C:158:HIS:HB2	1:C:160:HIS:ND1	2.27	0.49
1:B:119:HIS:NE2	1:B:254:LYS:HD3	2.27	0.49
1:C:21:ASN:C	1:C:22(A):CYS:N	2.65	0.49
1:C:31:TYR:CE1	1:C:46:LYS:HG3	2.46	0.49
1:A:154:ALA:HB1	1:A:161:THR:HG21	1.95	0.49
1:A:60:LEU:CD1	1:A:125:ALA:HB1	2.42	0.49
1:A:49:LYS:O	1:A:160:HIS:NE2	2.46	0.48
1:B:156:ARG:O	1:B:157:PHE:C	2.51	0.48
1:B:21:ASN:HB2	1:B:31:TYR:CE2	2.48	0.48
1:B:161:THR:OG1	1:B:162:THR:N	2.46	0.48
1:B:54:ALA:HA	1:B:157:PHE:CE1	2.49	0.47
1:B:54:ALA:HA	1:B:157:PHE:CD2	2.49	0.47
1:B:173:MET:HB3	1:B:173:MET:HE2	1.78	0.47
1:B:21:ASN:HD21	1:B:25:GLY:H	1.62	0.47
1:B:57:LEU:CD1	1:B:153:GLY:HA3	2.45	0.47
1:C:54:ALA:HA	1:C:157:PHE:CE1	2.49	0.47
1:D:8:PHE:CZ	1:D:71:VAL:HG11	2.49	0.47
1:D:15:ASP:C	1:D:36:ILE:HD12	2.36	0.47
1:B:122:HIS:CE1	1:B:185:GLU:HB2	2.50	0.46
1:D:181:LEU:HB3	1:D:182:PRO:HD2	1.98	0.46
1:B:8:PHE:CZ	1:B:55:GLU:HG2	2.50	0.46
1:B:40:LYS:HA	1:B:40:LYS:HE2	1.97	0.46
1:D:210:GLU:HB2	1:D:213:GLN:OE1	2.15	0.46
1:C:280:LYS:HA	1:C:283:TRP:CE2	2.50	0.46
1:B:157:PHE:HE2	2:B:401:IGS:C47	2.29	0.45
1:D:56:ILE:O	1:D:59:VAL:HG22	2.16	0.45
1:C:52:LYS:C	1:C:54:ALA:N	2.70	0.45
1:C:80:ILE:HD13	2:C:401:IGS:C51	2.45	0.45
1:A:21:ASN:HB3	1:A:31:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HB3	1:A:182:PRO:HD2	2.00	0.44
1:B:54:ALA:HA	1:B:157:PHE:CZ	2.52	0.44
1:C:21:ASN:CA	1:C:22(A):CYS:N	2.80	0.44
1:A:53:GLU:HB3	1:A:157:PHE:HE1	1.82	0.44
1:D:49:LYS:HD2	1:D:51:GLU:OE1	2.17	0.44
1:D:64:ASN:C	1:D:65:ILE:HD12	2.37	0.44
1:B:51:GLU:O	1:B:54:ALA:HB3	2.17	0.44
1:B:158:HIS:HB2	1:B:161:THR:HG22	1.99	0.44
1:B:181:LEU:HD12	1:B:181:LEU:HA	1.77	0.44
1:D:128:LYS:HB2	1:D:128:LYS:HE2	1.83	0.44
1:C:57:LEU:HA	1:C:60:LEU:HG	1.98	0.44
1:D:228:PRO:HB3	1:D:283:TRP:HB2	1.99	0.43
1:B:52:LYS:C	1:B:54:ALA:N	2.69	0.43
1:A:158:HIS:HB2	1:A:160:HIS:CE1	2.53	0.43
1:B:268:SER:O	1:B:272:LYS:HG3	2.18	0.43
1:C:45:LYS:HE3	2:C:401:IGS:C05	2.49	0.43
1:D:56:ILE:HD13	1:D:127:VAL:CG1	2.48	0.43
1:B:21:ASN:HD21	1:B:24:GLY:H	1.66	0.43
1:C:54:ALA:HA	1:C:157:PHE:CD1	2.54	0.43
1:C:54:ALA:C	1:C:157:PHE:CZ	2.92	0.43
1:A:210:GLU:HB2	1:A:213:GLN:CG	2.42	0.43
1:C:157:PHE:HB3	1:C:158:HIS:H	1.59	0.43
1:B:131:HIS:O	1:B:132:ARG:HB2	2.19	0.42
1:A:54:ALA:HA	1:A:157:PHE:CD1	2.54	0.42
1:C:135:LYS:HE2	1:C:138:ASN:ND2	2.35	0.42
1:C:156:ARG:HG3	1:C:157:PHE:HD1	1.84	0.42
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.92	0.42
1:D:17:GLN:HG3	1:D:36:ILE:HD11	2.01	0.42
1:D:47:LEU:HD11	1:D:80:ILE:HD11	2.00	0.42
1:B:157:PHE:HB3	1:B:158:HIS:H	1.49	0.42
1:C:54:ALA:HA	1:C:157:PHE:CG	2.54	0.42
1:B:56:ILE:O	1:B:59:VAL:HG22	2.20	0.42
1:D:12:LYS:HG2	3:D:533:HOH:O	2.20	0.42
1:B:99:SER:OG	1:B:202:ARG:NE	2.41	0.42
1:B:157:PHE:CE2	2:B:401:IGS:C47	3.03	0.42
1:B:54:ALA:HA	1:B:157:PHE:CE2	2.55	0.41
1:C:156:ARG:HG3	1:C:157:PHE:N	2.35	0.41
1:A:166:LEU:HD22	1:A:166:LEU:HA	1.71	0.41
1:B:132:ARG:HD2	1:B:155:SER:HB2	2.03	0.41
1:B:167:VAL:HG13	1:B:211:GLY:HA3	2.02	0.41
1:A:273:CYS:O	1:A:277:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLU:O	1:C:213:GLN:HB3	2.21	0.40
1:B:57:LEU:HD12	1:B:157:PHE:CE2	2.56	0.40
1:A:246:ASP:OD1	1:A:248:LYS:HE3	2.21	0.40
1:D:8:PHE:CE2	1:D:71:VAL:HG21	2.56	0.40
1:B:166:LEU:HG	1:B:170:PHE:CZ	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:SER:N	1:A:220:GLU:OE2[2_554]	0.99	1.21
1:D:165:SER:CA	1:A:220:GLU:OE2[2_554]	1.73	0.47
1:D:165:SER:N	1:A:220:GLU:CD[2_554]	2.11	0.09

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	288/310 (93%)	279 (97%)	7 (2%)	2 (1%)	22	18
1	B	288/310 (93%)	278 (96%)	7 (2%)	3 (1%)	15	11
1	C	286/310 (92%)	275 (96%)	10 (4%)	1 (0%)	41	41
1	D	288/310 (93%)	281 (98%)	6 (2%)	1 (0%)	41	41
All	All	1150/1240 (93%)	1113 (97%)	30 (3%)	7 (1%)	25	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	158	HIS
1	A	52	LYS
1	A	162	THR

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Mol	Chain	Res	Type
1	B	19	PHE
1	B	161	THR
1	C	54	ALA
1	B	157	PHE

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	255/274 (93%)	246 (96%)	9 (4%)	36	38
1	B	255/274 (93%)	245 (96%)	10 (4%)	32	33
1	C	255/274 (93%)	246 (96%)	9 (4%)	36	38
1	D	255/274 (93%)	246 (96%)	9 (4%)	36	38
All	All	1020/1096 (93%)	983 (96%)	37 (4%)	35	36

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

Mol	Chain	Res	Type
1	D	8	PHE
1	D	157	PHE
1	D	158	HIS
1	D	159	ASN
1	D	160	HIS
1	D	161	THR
1	D	166	LEU
1	D	233	ARG
1	D	275	SER
1	A	21	ASN
1	A	34	LYS
1	A	52	LYS
1	A	98	ARG
1	A	161	THR
1	A	166	LEU
1	A	167	VAL
1	A	233	ARG

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Mol	Chain	Res	Type
1	A	248	LYS
1	B	40	LYS
1	B	46	LYS
1	B	49	LYS
1	B	127	VAL
1	B	156	ARG
1	B	158	HIS
1	B	161	THR
1	B	181	LEU
1	B	233	ARG
1	B	279	ASN
1	C	8	PHE
1	C	27	PHE
1	C	60	LEU
1	C	83	GLU
1	C	97	ASN
1	C	161	THR
1	C	162	THR
1	C	233	ARG
1	C	275	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	138	ASN
1	D	222	ASN
1	B	21	ASN
1	B	240	HIS

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

4 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
2	IGS	C	401	1	50,52,52	1.93	9 (18%)	57,74,74	2.91	16 (28%)
2	IGS	D	401	1	50,52,52	1.83	10 (20%)	57,74,74	2.80	15 (26%)
2	IGS	B	401	1	50,52,52	1.85	8 (16%)	57,74,74	2.79	17 (29%)
2	IGS	A	401	1	50,52,52	1.80	10 (20%)	57,74,74	3.17	19 (33%)

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	IGS	C	401	1	-	3/29/33/33	0/6/6/6
2	IGS	D	401	1	-	5/29/33/33	0/6/6/6
2	IGS	B	401	1	-	3/29/33/33	0/6/6/6
2	IGS	A	401	1	-	2/29/33/33	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	IGS	O24-C23	7.10	1.41	1.35
2	C	401	IGS	O24-C23	6.96	1.41	1.35
2	B	401	IGS	C29-N28	6.45	1.48	1.33
2	C	401	IGS	C29-N28	6.32	1.47	1.33
2	A	401	IGS	C29-N28	6.10	1.47	1.33
2	B	401	IGS	O24-C23	5.99	1.40	1.35
2	A	401	IGS	O24-C23	5.88	1.40	1.35
2	D	401	IGS	C29-N28	5.86	1.46	1.33
2	C	401	IGS	C41-S02	4.03	1.82	1.76
2	B	401	IGS	O53-S02	3.94	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	IGS	C41-S02	3.88	1.82	1.76
2	D	401	IGS	C41-S02	3.66	1.82	1.76
2	B	401	IGS	C41-S02	3.64	1.82	1.76
2	B	401	IGS	N11-N10	-3.58	1.31	1.37
2	C	401	IGS	O53-S02	3.57	1.47	1.43
2	D	401	IGS	O01-S02	3.32	1.47	1.43
2	C	401	IGS	S02-N03	3.26	1.69	1.63
2	A	401	IGS	O53-S02	3.23	1.47	1.43
2	B	401	IGS	O01-S02	2.94	1.46	1.43
2	A	401	IGS	C04-C39	-2.70	1.34	1.38
2	A	401	IGS	N11-N10	-2.65	1.33	1.37
2	D	401	IGS	N11-N10	-2.59	1.33	1.37
2	C	401	IGS	N11-N10	-2.58	1.33	1.37
2	D	401	IGS	O53-S02	2.57	1.46	1.43
2	C	401	IGS	O01-S02	2.57	1.46	1.43
2	A	401	IGS	C09-C39	-2.56	1.35	1.39
2	D	401	IGS	C15-C14	2.50	1.52	1.48
2	D	401	IGS	S02-N03	2.48	1.67	1.63
2	C	401	IGS	C46-C45	2.23	1.54	1.49
2	A	401	IGS	O01-S02	2.22	1.46	1.43
2	C	401	IGS	C09-C39	-2.19	1.36	1.39
2	B	401	IGS	S02-N03	2.16	1.67	1.63
2	A	401	IGS	C46-C45	2.13	1.54	1.49
2	B	401	IGS	C17-C20	-2.10	1.37	1.43
2	A	401	IGS	C15-C14	2.06	1.52	1.48
2	D	401	IGS	C23-C17	-2.03	1.43	1.45
2	D	401	IGS	O38-C29	-2.01	1.19	1.23

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	IGS	O53-S02-O01	-14.74	101.43	119.55
2	D	401	IGS	O53-S02-O01	-14.22	102.07	119.55
2	B	401	IGS	O53-S02-O01	-12.32	104.40	119.55
2	C	401	IGS	O53-S02-O01	-11.44	105.49	119.55
2	C	401	IGS	C07-C09-N10	8.13	125.15	117.84
2	C	401	IGS	C15-C18-N19	-7.77	118.36	125.55
2	A	401	IGS	C15-C18-N19	-7.35	118.74	125.55
2	B	401	IGS	C15-C18-N19	-7.20	118.88	125.55
2	B	401	IGS	C07-C09-N10	6.91	124.05	117.84
2	C	401	IGS	C41-S02-N03	6.66	115.21	106.83
2	A	401	IGS	C07-C09-N10	6.41	123.61	117.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	IGS	C41-S02-N03	6.30	114.75	106.83
2	D	401	IGS	C15-C18-N19	-6.12	119.88	125.55
2	C	401	IGS	C06-C07-C09	-5.10	118.58	123.89
2	D	401	IGS	O53-S02-C41	4.97	114.09	107.97
2	B	401	IGS	C16-C15-C18	4.74	122.86	116.24
2	A	401	IGS	C05-C04-N03	4.62	130.12	120.88
2	C	401	IGS	C07-C09-C39	4.60	121.24	115.66
2	C	401	IGS	C16-C15-C18	4.47	122.49	116.24
2	A	401	IGS	C18-N19-C20	4.42	121.14	116.69
2	D	401	IGS	C07-C09-C39	4.42	121.02	115.66
2	A	401	IGS	C16-C15-C18	4.36	122.34	116.24
2	C	401	IGS	C18-N19-C20	4.35	121.06	116.69
2	D	401	IGS	C30-C29-N28	4.26	120.29	115.79
2	D	401	IGS	C18-N19-C20	4.26	120.97	116.69
2	D	401	IGS	C09-C39-C04	-4.19	118.27	124.61
2	C	401	IGS	C05-C04-N03	4.14	129.16	120.88
2	B	401	IGS	C06-C07-C09	-4.08	119.65	123.89
2	A	401	IGS	C30-C29-N28	4.07	120.09	115.79
2	A	401	IGS	C07-C09-C39	4.04	120.56	115.66
2	B	401	IGS	C07-C09-C39	3.96	120.47	115.66
2	A	401	IGS	F08-C07-C09	-3.90	116.19	119.45
2	B	401	IGS	C18-N19-C20	3.89	120.61	116.69
2	B	401	IGS	C30-C29-N28	3.88	119.89	115.79
2	A	401	IGS	O01-S02-C41	3.80	112.65	107.97
2	A	401	IGS	C06-C07-C09	-3.79	119.95	123.89
2	B	401	IGS	C05-C04-N03	3.66	128.20	120.88
2	D	401	IGS	C16-C15-C18	3.61	121.29	116.24
2	B	401	IGS	C41-S02-N03	3.46	111.19	106.83
2	A	401	IGS	C05-C04-C39	3.44	122.87	117.80
2	D	401	IGS	C06-C07-C09	-3.44	120.31	123.89
2	D	401	IGS	C41-S02-N03	3.33	111.02	106.83
2	C	401	IGS	F08-C07-C09	-3.30	116.69	119.45
2	C	401	IGS	C30-C29-N28	3.30	119.28	115.79
2	B	401	IGS	F08-C07-C09	-3.04	116.91	119.45
2	A	401	IGS	C09-C39-C04	-2.93	120.17	124.61
2	A	401	IGS	C52-C41-S02	-2.85	115.88	119.08
2	B	401	IGS	C15-C16-C17	-2.82	116.13	122.30
2	B	401	IGS	O53-S02-C41	2.80	111.42	107.97
2	A	401	IGS	C42-C41-S02	2.79	122.81	119.77
2	C	401	IGS	F08-C07-C06	2.75	124.73	118.59
2	A	401	IGS	C15-C16-C17	-2.57	116.67	122.30
2	D	401	IGS	F40-C39-C04	2.55	122.53	118.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	IGS	C05-C04-C39	2.49	121.47	117.80
2	D	401	IGS	C15-C16-C17	-2.49	116.85	122.30
2	B	401	IGS	C09-C39-C04	-2.49	120.84	124.61
2	C	401	IGS	C15-C16-C17	-2.44	116.96	122.30
2	A	401	IGS	F08-C07-C06	2.36	123.86	118.59
2	D	401	IGS	C52-C41-S02	2.34	121.70	119.08
2	C	401	IGS	C09-C39-C04	-2.25	121.21	124.61
2	D	401	IGS	C25-O24-C23	-2.21	113.37	117.51
2	B	401	IGS	F08-C07-C06	2.18	123.45	118.59
2	A	401	IGS	O01-S02-N03	2.17	112.16	106.73
2	B	401	IGS	C09-N10-N11	2.15	121.33	117.84
2	D	401	IGS	C44-C45-C52	2.12	121.16	118.16
2	C	401	IGS	C09-N10-N11	2.09	121.22	117.84
2	C	401	IGS	C42-C41-S02	2.08	122.03	119.77

There are no chirality outliers.

All (13) torsion outliers are listed below:

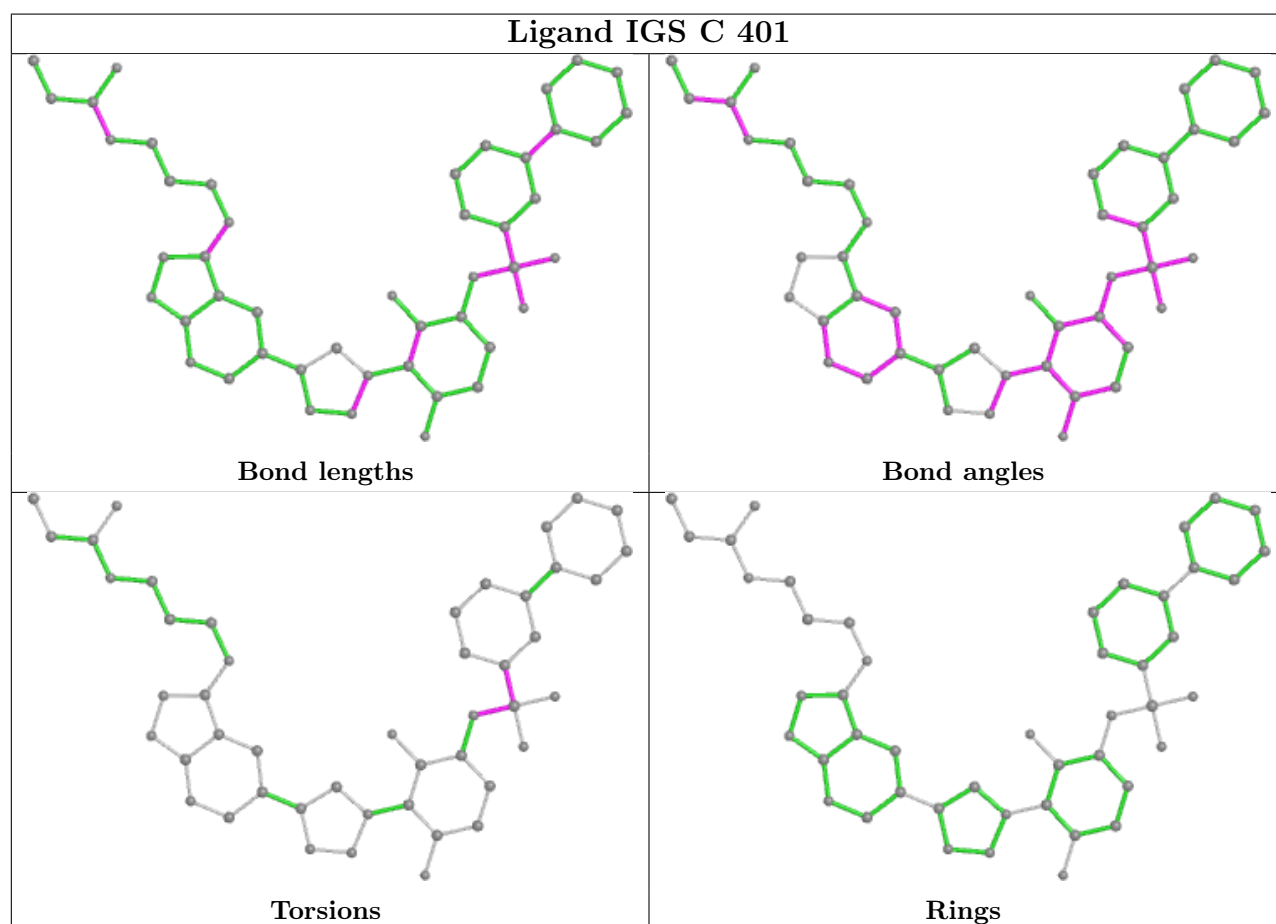
Mol	Chain	Res	Type	Atoms
2	D	401	IGS	C25-C26-C27-N28
2	D	401	IGS	O24-C25-C26-C27
2	A	401	IGS	C42-C41-S02-O01
2	A	401	IGS	C52-C41-S02-O01
2	B	401	IGS	C42-C41-S02-O01
2	B	401	IGS	C52-C41-S02-O01
2	D	401	IGS	C52-C41-S02-O53
2	C	401	IGS	C42-C41-S02-O01
2	D	401	IGS	C42-C41-S02-O53
2	D	401	IGS	C39-C09-N10-N11
2	C	401	IGS	C52-C41-S02-O01
2	B	401	IGS	C25-C26-C27-N28
2	C	401	IGS	C04-N03-S02-O53

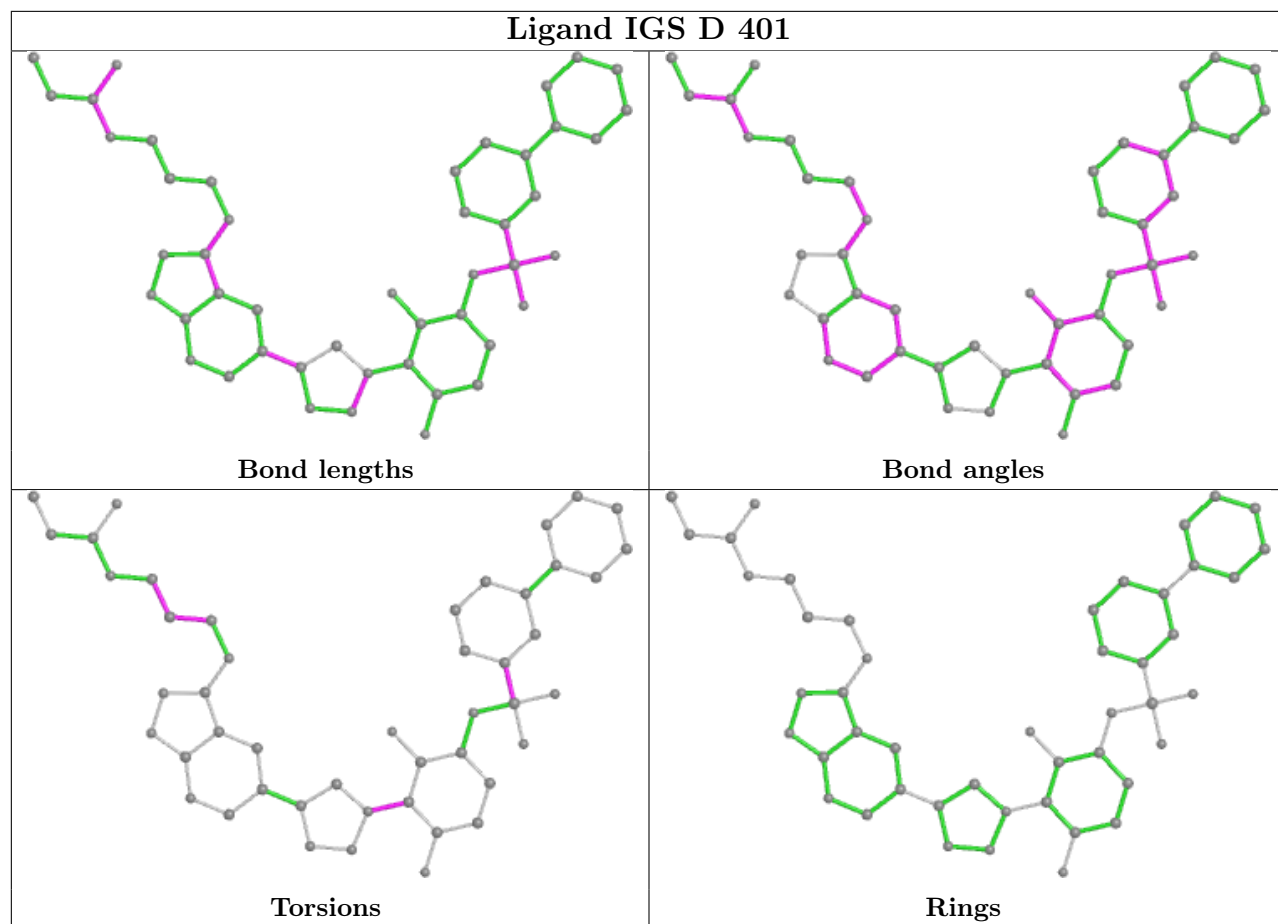
There are no ring outliers.

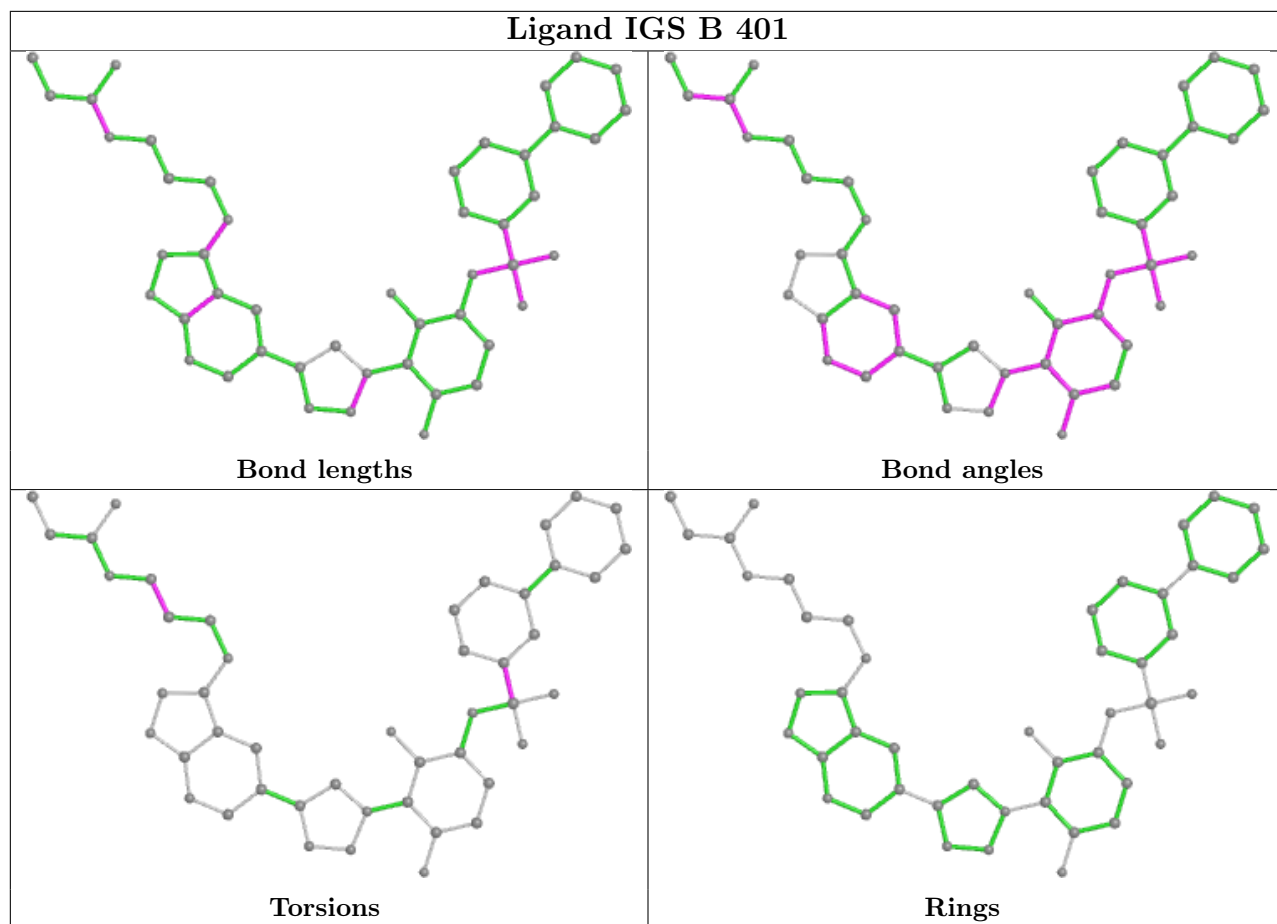
3 monomers are involved in 6 short contacts:

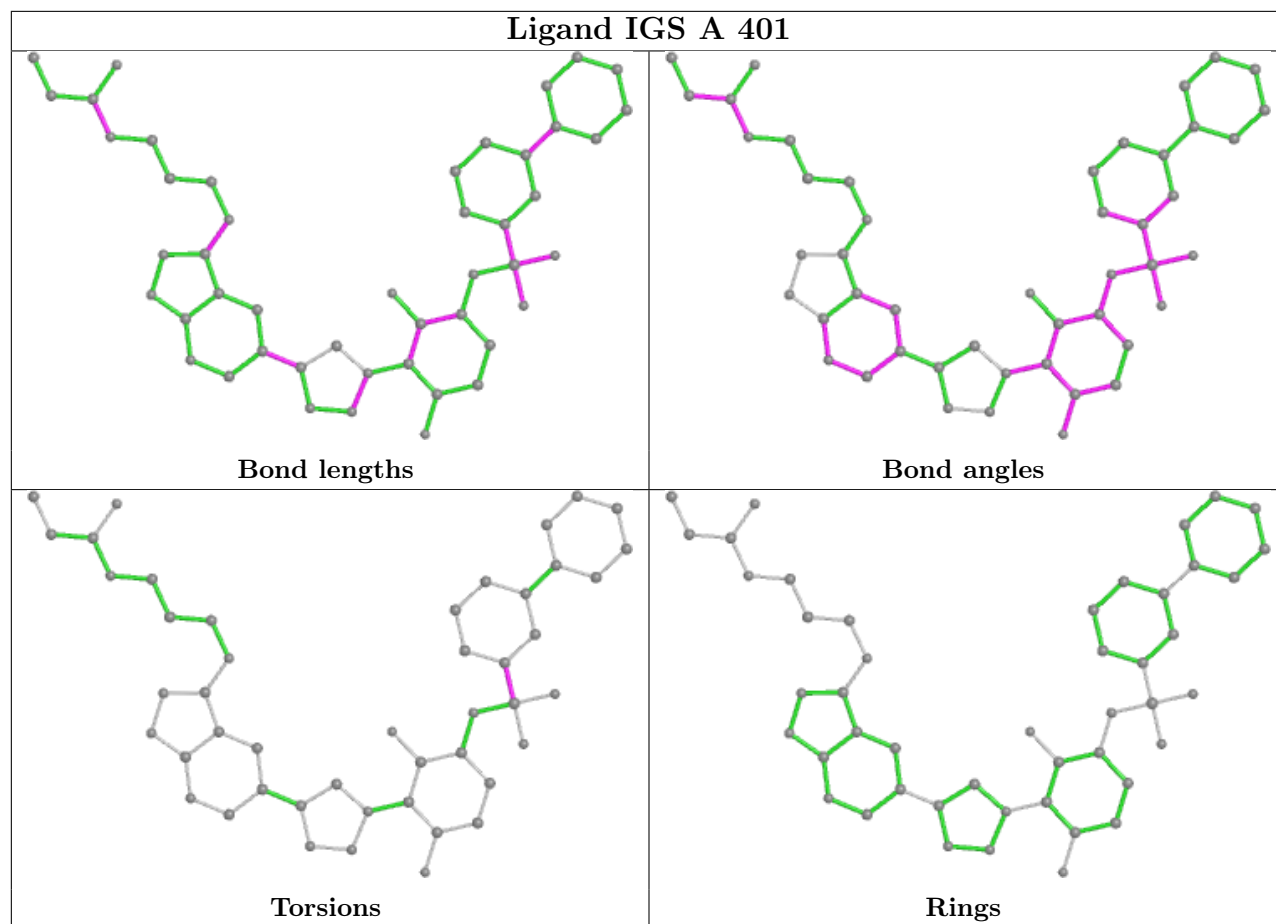
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	IGS	3	0
2	D	401	IGS	1	0
2	B	401	IGS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	21:ASN	C	22(A):CYS	N	2.65

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	291/310 (93%)	0.26	21 (7%) 15 19	17, 30, 61, 78	0
1	B	291/310 (93%)	0.39	24 (8%) 11 15	17, 29, 65, 90	0
1	C	291/310 (93%)	0.40	28 (9%) 8 10	19, 31, 69, 100	0
1	D	291/310 (93%)	0.59	32 (10%) 5 7	20, 37, 64, 90	0
All	All	1164/1240 (93%)	0.41	105 (9%) 9 12	17, 32, 65, 100	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	161	THR	17.3
1	B	157	PHE	16.9
1	B	54	ALA	14.3
1	C	157	PHE	14.2
1	D	157	PHE	11.0
1	C	162	THR	10.5
1	A	160	HIS	10.1
1	B	161	THR	10.0
1	D	167	VAL	9.0
1	D	163	HIS	8.8
1	C	163	HIS	8.7
1	C	160	HIS	8.2
1	D	166	LEU	8.1
1	B	162	THR	8.0
1	D	160	HIS	8.0
1	D	161	THR	7.8
1	C	158	HIS	7.8
1	B	158	HIS	7.5
1	A	24	GLY	7.3
1	A	165	SER	7.1
1	D	158	HIS	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	160	HIS	6.8
1	C	54	ALA	6.8
1	D	162	THR	6.7
1	B	163	HIS	6.6
1	D	159	ASN	6.5
1	B	167	VAL	6.2
1	C	299	ARG	6.1
1	A	161	THR	6.1
1	A	166	LEU	6.0
1	B	159	ASN	5.8
1	C	24	GLY	5.6
1	A	297	LEU	5.6
1	A	163	HIS	5.6
1	C	167	VAL	5.5
1	A	157	PHE	5.3
1	D	165	SER	5.1
1	C	216	TRP	5.0
1	B	27	PHE	4.8
1	A	26	SER	4.8
1	C	159	ASN	4.8
1	A	159	ASN	4.7
1	A	299	ARG	4.7
1	C	27	PHE	4.6
1	C	25	GLY	4.6
1	C	298	GLU	4.6
1	A	25	GLY	4.5
1	A	162	THR	4.2
1	B	25	GLY	3.9
1	B	24	GLY	3.8
1	A	158	HIS	3.8
1	D	296	LYS	3.8
1	B	22(A)	CYS	3.6
1	C	26	SER	3.5
1	B	166	LEU	3.5
1	C	166	LEU	3.5
1	D	299	ARG	3.2
1	A	97	ASN	3.2
1	C	180	SER	3.1
1	D	51	GLU	3.1
1	C	212	LEU	3.1
1	D	27	PHE	3.1
1	A	167	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	292	GLU	3.1
1	D	297	LEU	3.0
1	B	212	LEU	3.0
1	A	27	PHE	3.0
1	D	8	PHE	2.9
1	D	53	GLU	2.9
1	B	154	ALA	2.8
1	A	298	GLU	2.8
1	D	54	ALA	2.8
1	B	216	TRP	2.8
1	D	295	LYS	2.7
1	B	165	SER	2.7
1	C	155	SER	2.6
1	B	182	PRO	2.6
1	D	23	GLY	2.5
1	A	23	GLY	2.5
1	C	165	SER	2.5
1	B	298	GLU	2.4
1	C	278	HIS	2.4
1	D	97	ASN	2.4
1	B	26	SER	2.4
1	C	195	VAL	2.4
1	C	57	LEU	2.3
1	D	24	GLY	2.3
1	C	48	LEU	2.3
1	B	156	ARG	2.3
1	D	291	LEU	2.3
1	A	48	LEU	2.2
1	D	195	VAL	2.2
1	C	97	ASN	2.2
1	D	281	ALA	2.2
1	C	28	GLY	2.2
1	D	26	SER	2.2
1	C	22(A)	CYS	2.1
1	D	278	HIS	2.1
1	B	23	GLY	2.1
1	D	156	ARG	2.1
1	B	267	THR	2.1
1	A	296	LYS	2.1
1	D	155	SER	2.0
1	D	139	VAL	2.0
1	D	134	LEU	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](#)

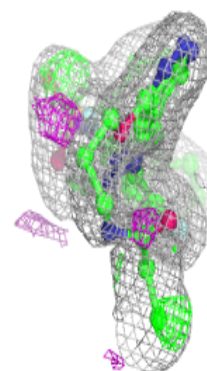
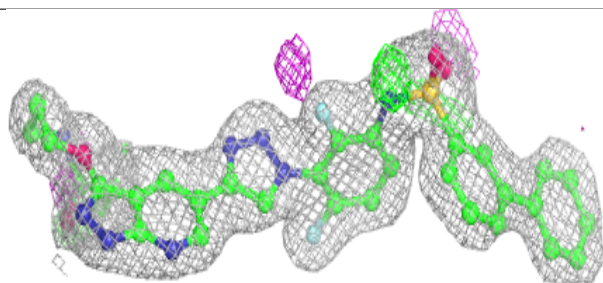
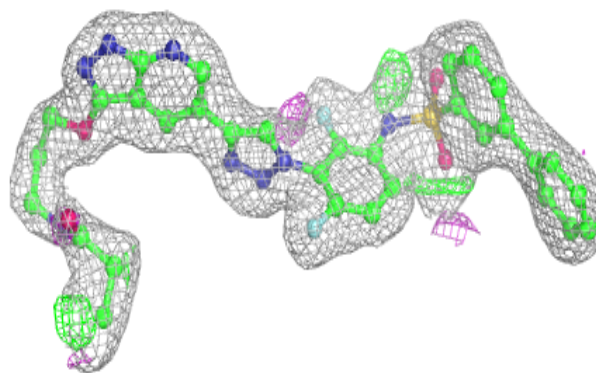
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IGS	C	401	47/47	0.91	0.12	23,33,46,50	0
2	IGS	B	401	47/47	0.93	0.13	21,28,47,51	0
2	IGS	D	401	47/47	0.94	0.13	23,36,55,59	0
2	IGS	A	401	47/47	0.96	0.10	19,26,41,47	0

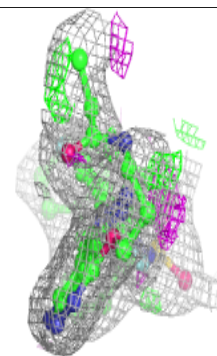
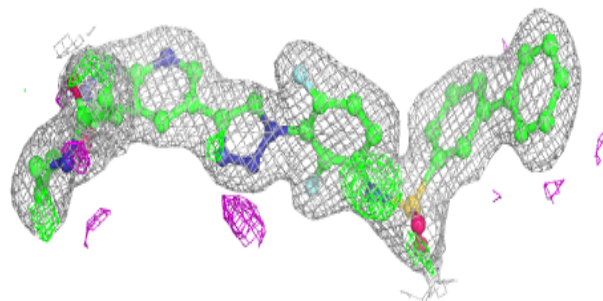
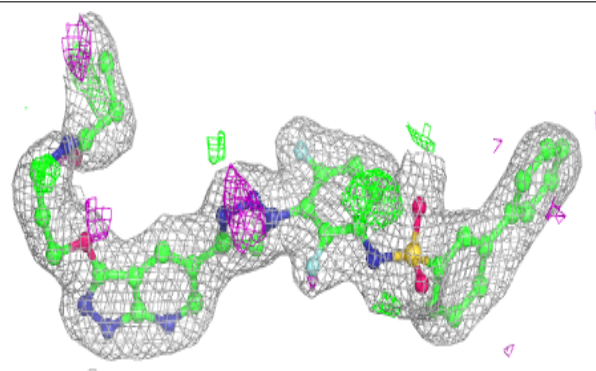
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IGS C 401:

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

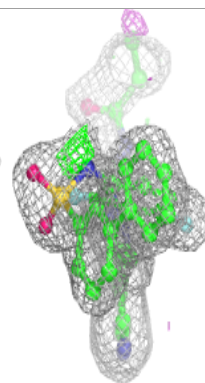
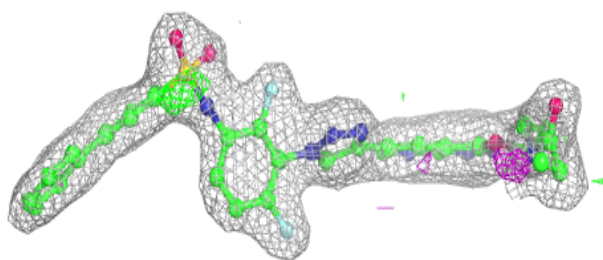
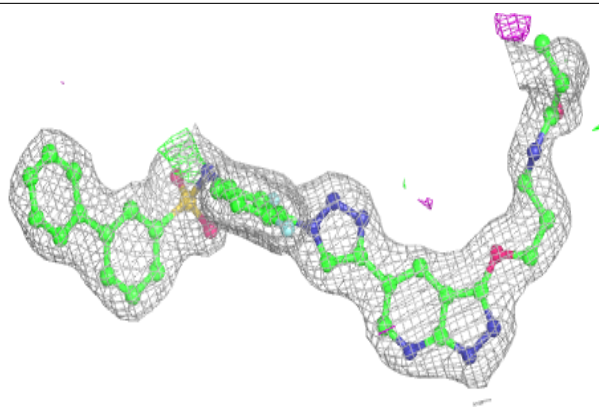
**Electron density around IGS B 401:**

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

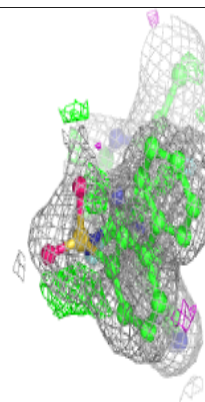
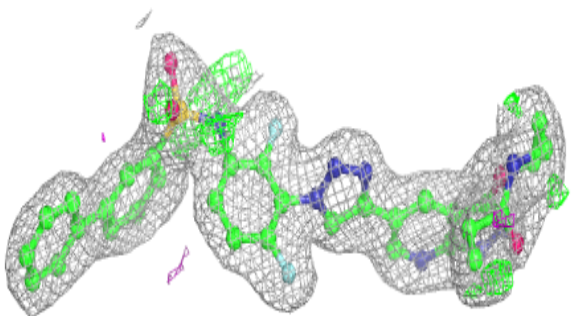
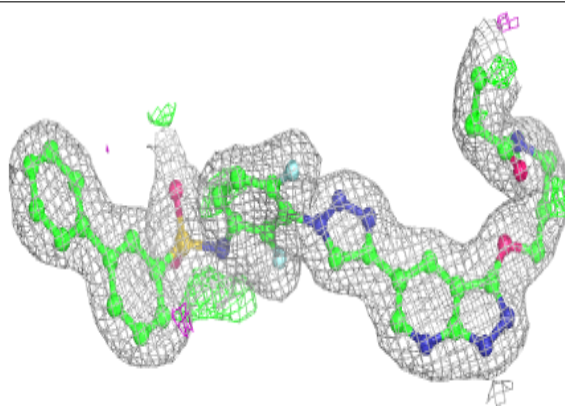


Electron density around IGS D 401:

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

**Electron density around IGS A 401:**

$2mF_o-DF_c$ (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.