Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 11:58 AM EDT

PDB ID	:	7RS4
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-8
Authors	:	Min, J.; Nwachukwu, J.C.; Min, C.K.; Njeri, J.W.; Srinivasan, S.; Rangarajan, E.S.; Nettles, C.C.; Yan, S.; Houtman, R.; Griffin, P.R.; Izard, T.; Katzenellenbogen, B.S.; Katzenellenbogen, J.A.; Nettles, K.W.
Deposited on	:	2021-08-10
Resolution	:	1.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

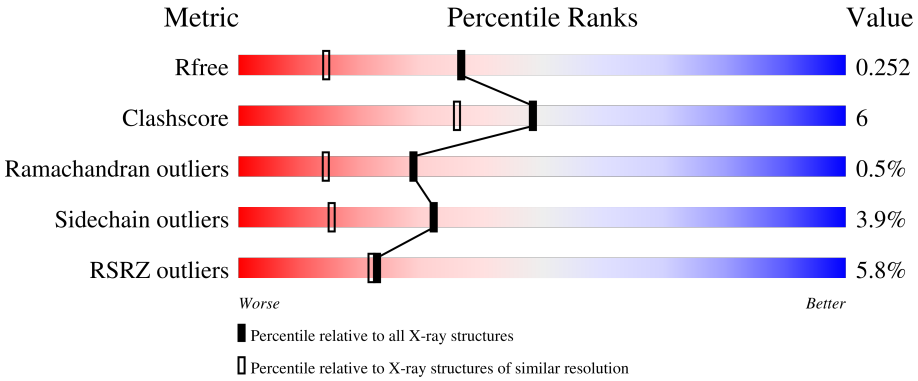
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	257	4% 84% 10% • 5%
1	B	257	7% 81% 13% • •
1	C	257	4% 83% 10% • 5%
1	D	257	7% 79% 15% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8147 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.

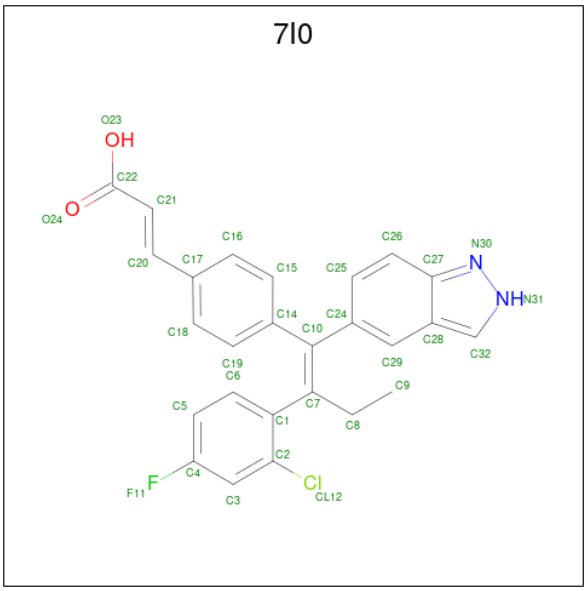
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	1	0
			1956	1249	333	356	18			
1	B	246	Total	C	N	O	S	0	0	0
			1965	1254	337	355	19			
1	C	244	Total	C	N	O	S	0	0	0
			1944	1242	330	353	19			
1	D	243	Total	C	N	O	S	0	0	0
			1947	1245	336	347	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	SER	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	372	SER	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	372	SER	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is (2E)-3-{4-[(1E)-2-(2-chloro-4-fluorophenyl)-1-(2H-indazol-5-yl)but-1-en-1-yl]phenyl}prop-2-enoic acid (three-letter code: 7I0) (formula: $C_{26}H_{20}ClFN_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C Cl F N O 32 26 1 1 2 2	0	0
2	B	1	Total C Cl F N O 32 26 1 1 2 2	0	0
2	C	1	Total C Cl F N O 32 26 1 1 2 2	0	0
2	D	1	Total C Cl F N O 32 26 1 1 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	49	Total O 49 49	0	0
4	C	63	Total O 63 63	0	0

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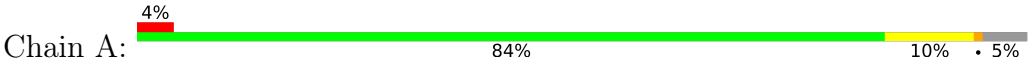
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	49	Total O 49 49	0	0

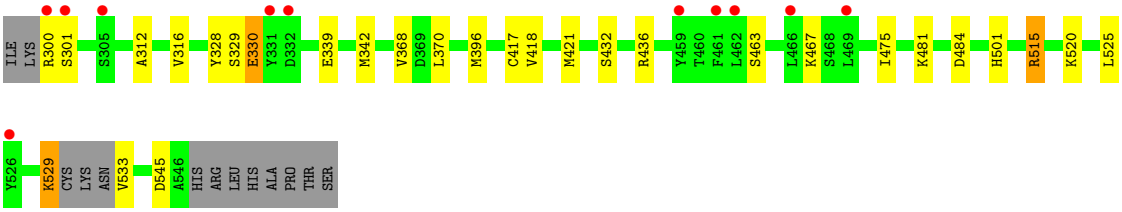
3 Residue-property plots (i)

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: Estrogen receptor

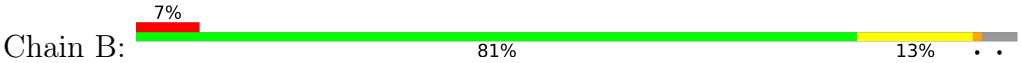
Chain A:

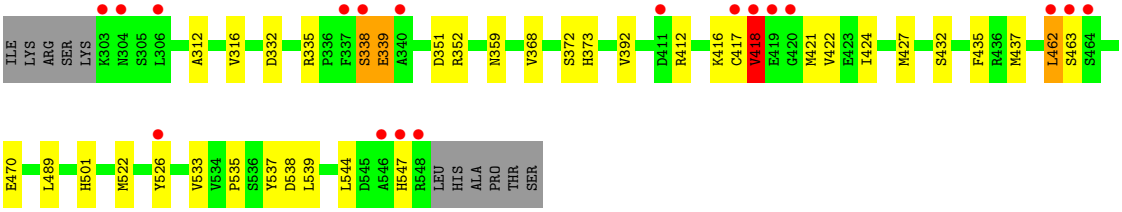




• Molecule 1: Estrogen receptor

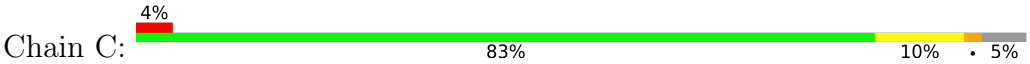
Chain B:

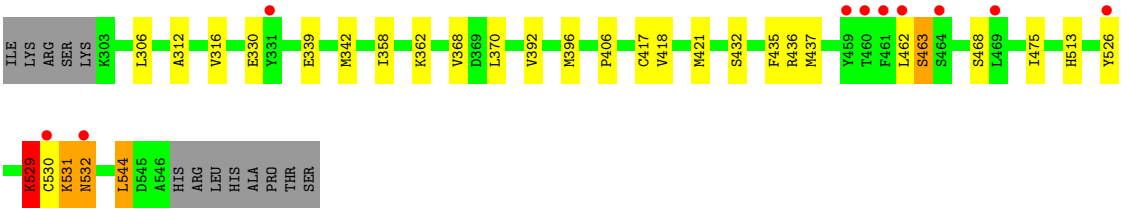




• Molecule 1: Estrogen receptor

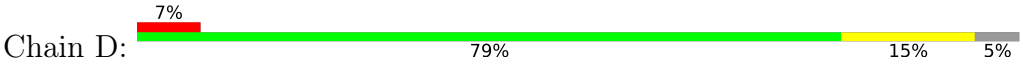
Chain C:

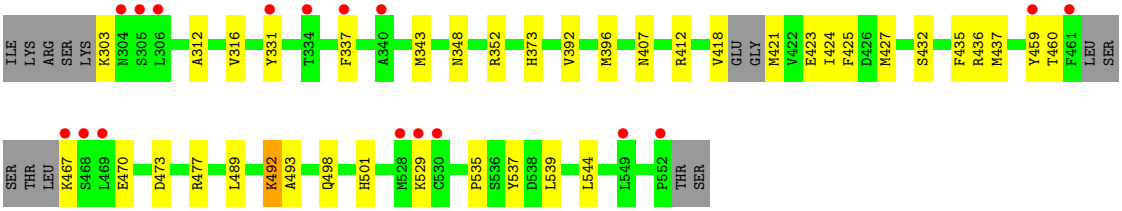




• Molecule 1: Estrogen receptor

Chain D:




ILE
LYS
ARG
SER
LYS
K303
N304
S305
L306
A312
V316
Y331
T334
F337
A340
M343
N348
R352
H373
V392
M396
N407
R412
V418
GLU
GLY
M421
V422
E423
I424
F425
D426
M427
S432
F435
R436
M437
Y459
T460
F461
LEU
SER

SER
THR
LEU
K467
S468
L469
E470
D473
R477
L489
K492
A493
Q498
H501
M528
K529
C530
P535
S536
Y537
D538
L539
L544
L549
P552
THR
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.09Å 58.82Å 93.71Å 86.88° 75.21° 63.40°	Depositor
Resolution (Å)	90.39 – 1.78 90.39 – 1.78	Depositor EDS
% Data completeness (in resolution range)	53.0 (90.39-1.78) 53.0 (90.39-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.251 0.205 , 0.252	Depositor DCC
R_{free} test set	2474 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.125 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8147	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 7I0, YCM

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	0.50	0/1980	0.69	1/2671 (0.0%)
1	B	0.49	0/1991	0.71	0/2688
1	C	0.49	0/1969	0.71	0/2659
1	D	0.49	0/1973	0.68	0/2662
All	All	0.49	0/7913	0.70	1/10680 (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	B	0	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	515	ARG	NE-CZ-NH1	5.56	123.08	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	338	SER	Peptide
1	C	529	LYS	Peptide
1	C	530	CYS	Peptide

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	1956	0	2002	18	2
1	B	1965	0	2011	29	2
1	C	1944	0	1991	28	0
1	D	1947	0	1991	27	0
2	A	32	0	0	0	0
2	B	32	0	0	2	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	B	1	0	0	1	0
3	D	1	0	0	0	0
4	A	44	0	0	6	0
4	B	49	0	0	2	0
4	C	63	0	0	3	0
4	D	49	0	0	3	0
All	All	8147	0	7995	95	2

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 6.

All (95) 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:501:HIS:HE1	4:A:742:HOH:O	1.50	0.94
1:D:343:MET:HG2	1:D:418:VAL:HG21	1.59	0.83
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.63	0.81
1:D:459:TYR:OH	4:D:701:HOH:O	1.99	0.80
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.65	0.78
1:A:525:LEU:HD13	1:A:533:VAL:HG11	1.65	0.78
1:B:417:CYS:O	1:B:418:VAL:HG13	1.85	0.77
1:C:342:MET:HE2	1:C:417:CYS:HB3	1.68	0.76
1:C:463:SER:OG	4:C:701:HOH:O	1.72	0.76
1:B:437:MET:HG3	4:B:748:HOH:O	1.85	0.75
1:C:463:SER:HB3	1:C:468:SER:HB2	1.70	0.73
1:B:338:SER:O	1:B:339:GLU:HG3	1.89	0.73
1:A:545:ASP:OD2	4:A:701:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:HIS:CD2	1:D:459:TYR:HD2	2.11	0.68
1:C:406:PRO:O	4:C:702:HOH:O	2.13	0.65
1:B:533:VAL:HG22	2:B:602:7I0:C21	2.28	0.64
1:A:501:HIS:CE1	4:A:742:HOH:O	2.35	0.64
1:C:532:ASN:CG	1:C:532:ASN:O	2.37	0.62
1:A:368:VAL:HG22	4:A:718:HOH:O	2.00	0.61
1:B:359:ASN:OD1	1:B:547:HIS:CE1	2.54	0.61
1:A:396:MET:O	1:A:436:ARG:HD3	2.01	0.60
1:C:396:MET:O	1:C:436:ARG:HD3	2.02	0.60
1:A:484:ASP:OD1	1:B:501:HIS:HE1	1.84	0.60
1:D:396:MET:O	1:D:436:ARG:HD3	2.02	0.60
1:D:489:LEU:O	1:D:492:LYS:HE3	2.03	0.59
1:A:418:VAL:CG1	1:A:421:MET:HE3	2.34	0.58
1:A:418:VAL:HG11	1:A:421:MET:HE3	1.84	0.57
1:C:531:LYS:HG3	1:C:532:ASN:H	1.68	0.57
4:A:742:HOH:O	1:B:501:HIS:HD2	1.87	0.56
1:B:338:SER:O	1:B:339:GLU:CG	2.53	0.56
1:B:332:ASP:HB3	1:B:335:ARG:HG2	1.88	0.55
1:D:535:PRO:HA	1:D:539:LEU:HD23	1.90	0.54
1:D:348:ASN:ND2	1:D:352:ARG:HH21	2.05	0.53
1:B:462:LEU:HD13	1:B:462:LEU:O	2.08	0.53
1:C:418:VAL:HG22	1:C:421:MET:HB2	1.91	0.53
1:B:338:SER:O	1:B:339:GLU:CB	2.57	0.53
1:A:418:VAL:HG22	1:A:421:MET:HB2	1.92	0.52
1:A:342:MET:CE	1:A:417:CYS:HB3	2.39	0.52
1:B:535:PRO:HA	1:B:539:LEU:HD23	1.91	0.52
1:C:513:HIS:CD2	1:D:459:TYR:CD2	2.96	0.52
1:C:532:ASN:O	1:C:532:ASN:ND2	2.43	0.52
1:D:492:LYS:HD2	1:D:492:LYS:C	2.30	0.52
1:A:342:MET:HE2	1:A:417:CYS:HB3	1.91	0.51
1:C:513:HIS:CE1	1:D:459:TYR:CE2	2.99	0.51
1:B:417:CYS:O	1:B:418:VAL:CG1	2.58	0.51
1:C:342:MET:CE	1:C:417:CYS:HB3	2.39	0.51
1:C:531:LYS:HG3	1:C:532:ASN:N	2.25	0.51
1:D:467:LYS:HB2	4:D:720:HOH:O	2.12	0.50
1:D:418:VAL:HB	1:D:421:MET:SD	2.52	0.50
1:D:423:GLU:HG3	1:D:424:ILE:N	2.25	0.50
1:B:418:VAL:HG22	1:B:421:MET:HB2	1.94	0.50
1:C:362:LYS:HD3	1:C:544:LEU:HD12	1.94	0.50
1:D:373:HIS:CD2	1:D:537:TYR:OH	2.65	0.50
1:B:373:HIS:CD2	1:B:537:TYR:OH	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:ILE:HD13	1:D:427:MET:CE	2.43	0.49
1:C:342:MET:HE3	1:C:418:VAL:HG13	1.95	0.49
1:C:368:VAL:HG22	4:C:706:HOH:O	2.13	0.49
1:C:339:GLU:HG3	1:C:418:VAL:HB	1.94	0.48
1:B:424:ILE:HD13	1:B:427:MET:CE	2.43	0.48
1:C:342:MET:HE3	1:C:418:VAL:CG1	2.44	0.48
1:B:416:LYS:CG	1:B:422:VAL:HG11	2.43	0.47
1:C:513:HIS:CG	1:D:459:TYR:HD2	2.33	0.47
1:C:513:HIS:CE1	1:D:459:TYR:CD2	3.02	0.47
1:C:513:HIS:NE2	1:D:459:TYR:CD2	2.83	0.47
1:A:339:GLU:HG3	1:A:418:VAL:HB	1.96	0.47
1:B:462:LEU:C	1:B:462:LEU:HD22	2.36	0.46
1:B:533:VAL:HG22	2:B:602:7I0:C22	2.46	0.46
1:B:352:ARG:HD2	3:B:601:CL:CL	2.53	0.46
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.51	0.46
1:C:358:ILE:HG23	1:C:544:LEU:HD13	1.99	0.45
1:D:473:ASP:OD2	1:D:477:ARG:NH1	2.50	0.45
1:A:312:ALA:O	1:A:316:VAL:HG23	2.16	0.44
1:C:312:ALA:O	1:C:316:VAL:HG23	2.17	0.44
1:D:492:LYS:HD2	1:D:493:ALA:N	2.32	0.44
4:A:742:HOH:O	1:B:501:HIS:CD2	2.67	0.44
1:B:416:LYS:HG3	1:B:422:VAL:HG11	2.00	0.43
1:B:417:CYS:C	1:B:418:VAL:CG1	2.87	0.43
1:C:463:SER:CB	1:C:468:SER:HB2	2.45	0.43
1:A:529:LYS:N	1:A:529:LYS:HD3	2.35	0.42
1:B:522:MET:HG3	1:B:526:TYR:CE1	2.53	0.42
1:D:392:VAL:HG12	1:D:435:PHE:CD2	2.55	0.42
1:B:312:ALA:O	1:B:316:VAL:HG23	2.19	0.42
1:C:526:TYR:O	1:C:529:LYS:O	2.37	0.42
1:B:351:ASP:HB2	1:B:533:VAL:HG11	2.00	0.42
1:B:392:VAL:HG12	1:B:435:PHE:CD2	2.55	0.41
1:A:342:MET:HE3	1:A:418:VAL:HG13	2.02	0.41
1:D:489:LEU:O	1:D:492:LYS:HG3	2.20	0.41
1:B:368:VAL:HG22	4:B:710:HOH:O	2.21	0.41
1:D:316:VAL:HG21	1:D:489:LEU:HD21	2.01	0.41
1:D:312:ALA:O	1:D:316:VAL:HG23	2.20	0.41
1:D:331:TYR:OH	1:D:407:ASN:O	2.31	0.41
1:C:392:VAL:HG12	1:C:435:PHE:CD2	2.55	0.41
1:D:460:THR:HG23	4:D:726:HOH:O	2.22	0.40
1:A:329:SER:O	1:A:330:GLU:C	2.60	0.40
1:B:316:VAL:HG21	1:B:489:LEU:HD21	2.02	0.40

All (2) 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:A:328:TYR:OH	1:B:359:ASN:ND2[1_645]	2.05	0.15
1:A:481:LYS:NZ	1:B:538:ASP:OD2[1_655]	2.19	0.01

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	240/257 (93%)	237 (99%)	2 (1%)	1 (0%)	34 19
1	B	243/257 (95%)	237 (98%)	4 (2%)	2 (1%)	19 7
1	C	241/257 (94%)	236 (98%)	3 (1%)	2 (1%)	19 7
1	D	236/257 (92%)	233 (99%)	3 (1%)	0	100 100
All	All	960/1028 (93%)	943 (98%)	12 (1%)	5 (0%)	29 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	GLU
1	C	531	LYS
1	A	330	GLU
1	B	418	VAL
1	C	330	GLU

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	220/231 (95%)	212 (96%)	8 (4%)	35 18
1	B	221/231 (96%)	213 (96%)	8 (4%)	35 18
1	C	219/231 (95%)	211 (96%)	8 (4%)	34 17
1	D	218/231 (94%)	208 (95%)	10 (5%)	27 11
All	All	878/924 (95%)	844 (96%)	34 (4%)	32 15

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	ARG
1	A	301	SER
1	A	432	SER
1	A	463	SER
1	A	467	LYS
1	A	515	ARG
1	A	520	LYS
1	A	529	LYS
1	B	372	SER
1	B	412	ARG
1	B	418	VAL
1	B	432	SER
1	B	462	LEU
1	B	463	SER
1	B	470	GLU
1	B	544	LEU
1	C	306	LEU
1	C	432	SER
1	C	437	MET
1	C	462	LEU
1	C	463	SER
1	C	529	LYS
1	C	532	ASN
1	C	544	LEU
1	D	303	LYS
1	D	337	PHE
1	D	412	ARG
1	D	425	PHE
1	D	432	SER
1	D	437	MET
1	D	470	GLU
1	D	492	LYS
1	D	529	LYS

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Mol	Chain	Res	Type
1	D	544	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	488	HIS
1	A	501	HIS
1	B	373	HIS
1	B	398	HIS
1	B	501	HIS
1	B	547	HIS
1	C	398	HIS
1	C	413	ASN
1	C	513	HIS
1	C	532	ASN
1	D	348	ASN
1	D	373	HIS
1	D	398	HIS
1	D	439	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	YCM	C	381	1	7,9,10	0.44	0	4,10,12	0.40	0
1	YCM	D	381	1	7,9,10	0.43	0	4,10,12	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	YCM	A	381	1	7,9,10	0.44	0	4,10,12	0.48	0
1	YCM	B	381	1	7,9,10	0.44	0	4,10,12	0.45	0

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	YCM	C	381	1	-	1/6/8/10	-
1	YCM	D	381	1	-	1/6/8/10	-
1	YCM	A	381	1	-	1/6/8/10	-
1	YCM	B	381	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	381	YCM	SG-CD-CE-NZ2
1	B	381	YCM	SG-CD-CE-NZ2
1	C	381	YCM	SG-CD-CE-NZ2
1	D	381	YCM	SG-CD-CE-NZ2

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	7I0	A	601	-	33,35,35	2.89	10 (30%)	43,49,49	1.67	9 (20%)
2	7I0	D	602	-	33,35,35	3.06	10 (30%)	43,49,49	1.29	5 (11%)
2	7I0	C	601	-	33,35,35	2.99	13 (39%)	43,49,49	1.51	10 (23%)
2	7I0	B	602	-	33,35,35	2.96	11 (33%)	43,49,49	1.89	13 (30%)

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	7I0	A	601	-	-	1/23/23/23	0/4/4/4
2	7I0	D	602	-	-	0/23/23/23	0/4/4/4
2	7I0	C	601	-	-	0/23/23/23	0/4/4/4
2	7I0	B	602	-	-	0/23/23/23	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	7I0	C10-C7	9.29	1.53	1.35
2	A	601	7I0	C10-C7	9.17	1.53	1.35
2	B	602	7I0	C10-C7	8.35	1.51	1.35
2	D	602	7I0	C21-C20	7.70	1.53	1.33
2	C	601	7I0	C10-C7	7.65	1.50	1.35
2	C	601	7I0	C21-C20	7.59	1.52	1.33
2	A	601	7I0	C21-C20	6.84	1.50	1.33
2	C	601	7I0	C1-C7	-6.00	1.39	1.49
2	B	602	7I0	C24-C10	-5.94	1.39	1.49
2	C	601	7I0	C26-C27	-5.80	1.31	1.41
2	B	602	7I0	C21-C20	5.58	1.47	1.33
2	A	601	7I0	C1-C7	-5.57	1.40	1.49
2	B	602	7I0	C14-C10	-5.41	1.40	1.49
2	D	602	7I0	C1-C7	-5.41	1.40	1.49
2	B	602	7I0	C26-C27	-5.25	1.32	1.41
2	C	601	7I0	C24-C10	-5.19	1.40	1.49
2	B	602	7I0	C1-C7	-5.03	1.41	1.49
2	D	602	7I0	C14-C10	-4.99	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	7I0	C24-C10	-4.90	1.41	1.49
2	D	602	7I0	C24-C10	-4.77	1.41	1.49
2	D	602	7I0	C26-C27	-4.66	1.33	1.41
2	A	601	7I0	C14-C10	-4.48	1.41	1.49
2	A	601	7I0	C26-C27	-4.41	1.34	1.41
2	B	602	7I0	F11-C4	4.20	1.46	1.36
2	C	601	7I0	F11-C4	-3.74	1.27	1.36
2	C	601	7I0	C14-C10	-3.72	1.43	1.49
2	C	601	7I0	C32-C28	-3.45	1.33	1.40
2	D	602	7I0	C32-C28	-3.31	1.33	1.40
2	D	602	7I0	C29-C28	-3.21	1.34	1.42
2	A	601	7I0	C17-C20	-3.15	1.38	1.47
2	B	602	7I0	C29-C28	-3.07	1.35	1.42
2	A	601	7I0	C32-C28	-2.98	1.34	1.40
2	B	602	7I0	C32-C28	-2.95	1.34	1.40
2	D	602	7I0	N31-N30	-2.85	1.32	1.37
2	C	601	7I0	C29-C28	-2.83	1.35	1.42
2	C	601	7I0	C8-C7	2.81	1.57	1.51
2	D	602	7I0	C17-C20	-2.57	1.40	1.47
2	B	602	7I0	C17-C20	-2.45	1.40	1.47
2	A	601	7I0	O23-C22	-2.33	1.24	1.30
2	C	601	7I0	C17-C20	-2.28	1.40	1.47
2	C	601	7I0	O23-C22	-2.27	1.24	1.30
2	C	601	7I0	C21-C22	2.22	1.53	1.48
2	B	602	7I0	N31-N30	-2.05	1.33	1.37
2	A	601	7I0	C29-C28	-2.04	1.37	1.42

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602	7I0	C19-C14-C10	-4.61	113.60	120.91
2	A	601	7I0	C6-C5-C4	4.38	122.89	118.36
2	A	601	7I0	C3-C2-CL12	-3.82	112.33	118.49
2	A	601	7I0	C5-C4-C3	-3.66	118.53	123.29
2	B	602	7I0	C15-C14-C10	3.47	126.42	120.91
2	D	602	7I0	C2-C3-C4	3.43	120.04	117.73
2	B	602	7I0	C5-C4-C3	-3.43	118.84	123.29
2	A	601	7I0	C8-C7-C10	-3.33	119.99	123.47
2	B	602	7I0	C8-C7-C10	-3.17	120.16	123.47
2	B	602	7I0	C8-C7-C1	2.96	118.69	114.43
2	B	602	7I0	C14-C10-C7	-2.96	119.55	122.86
2	B	602	7I0	C6-C5-C4	2.95	121.41	118.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602	7I0	C2-C3-C4	2.88	119.67	117.73
2	A	601	7I0	C25-C24-C29	-2.83	115.86	119.23
2	C	601	7I0	C3-C2-CL12	-2.82	113.94	118.49
2	A	601	7I0	C2-C3-C4	2.75	119.58	117.73
2	C	601	7I0	C1-C2-CL12	2.73	125.04	121.00
2	C	601	7I0	C5-C4-C3	-2.70	119.79	123.29
2	C	601	7I0	C6-C5-C4	2.60	121.06	118.36
2	C	601	7I0	C2-C3-C4	2.56	119.45	117.73
2	D	602	7I0	C17-C20-C21	-2.50	121.18	126.91
2	B	602	7I0	C18-C17-C20	-2.40	112.65	121.29
2	B	602	7I0	F11-C4-C5	2.40	122.61	118.54
2	D	602	7I0	C8-C7-C10	-2.39	120.97	123.47
2	D	602	7I0	C5-C4-C3	-2.39	120.19	123.29
2	B	602	7I0	O23-C22-C21	2.34	124.98	116.27
2	B	602	7I0	C17-C20-C21	-2.32	121.59	126.91
2	C	601	7I0	C17-C20-C21	-2.32	121.60	126.91
2	B	602	7I0	O24-C22-C21	-2.31	113.78	120.99
2	A	601	7I0	C3-C2-C1	2.30	123.28	121.58
2	A	601	7I0	C1-C2-CL12	2.29	124.39	121.00
2	D	602	7I0	C14-C10-C7	-2.23	120.36	122.86
2	C	601	7I0	C18-C19-C14	2.15	123.28	120.78
2	C	601	7I0	O23-C22-O24	-2.12	118.27	122.67
2	A	601	7I0	C8-C7-C1	2.08	117.42	114.43
2	C	601	7I0	C8-C7-C1	2.05	117.37	114.43
2	C	601	7I0	F11-C4-C5	2.01	121.95	118.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	7I0	C1-C7-C8-C9

There are no ring outliers.

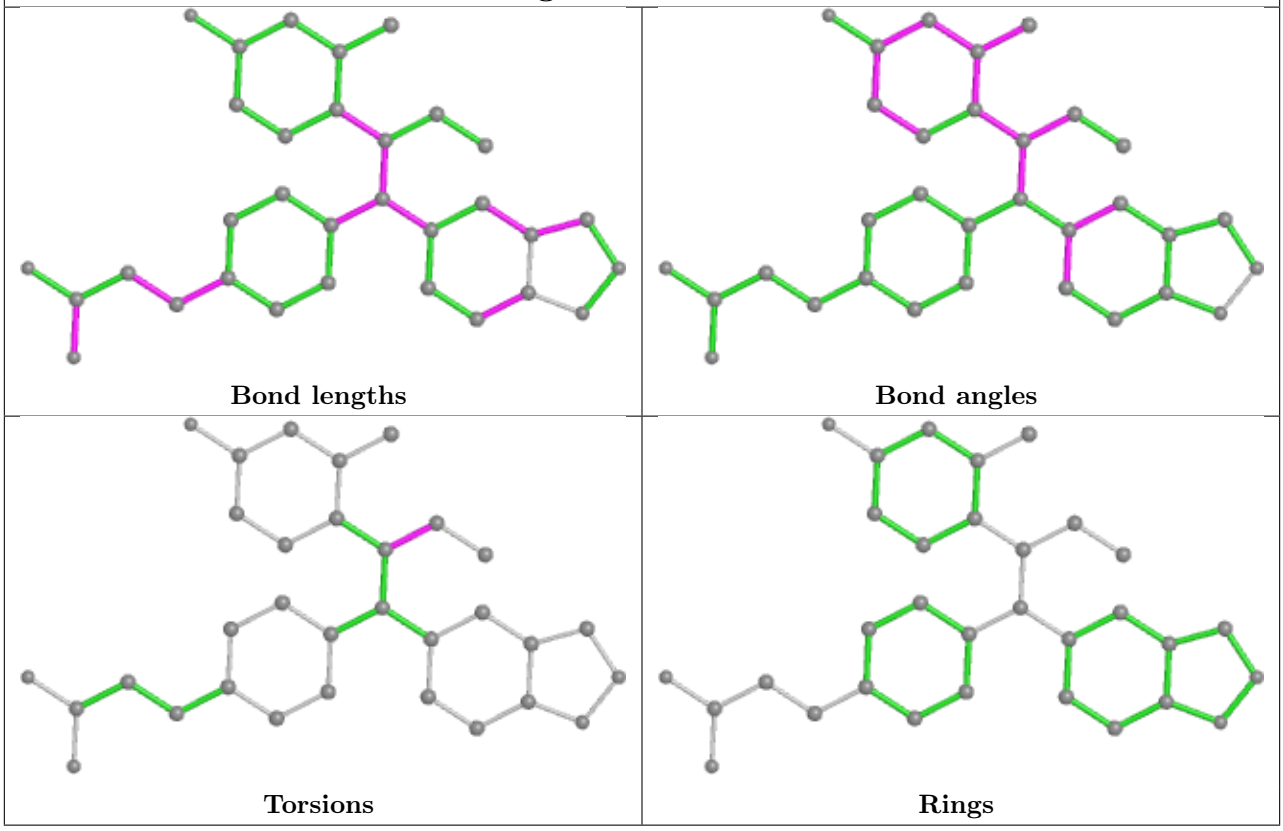
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	7I0	2	0

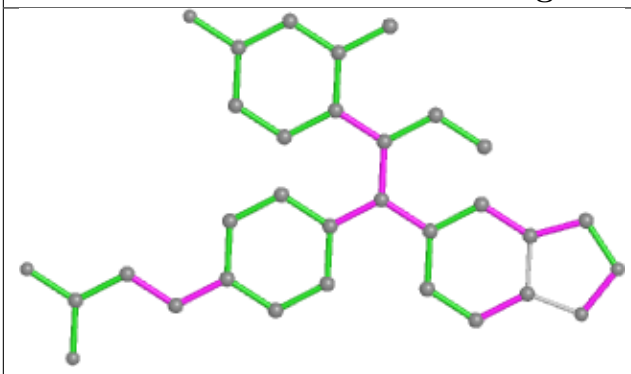
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

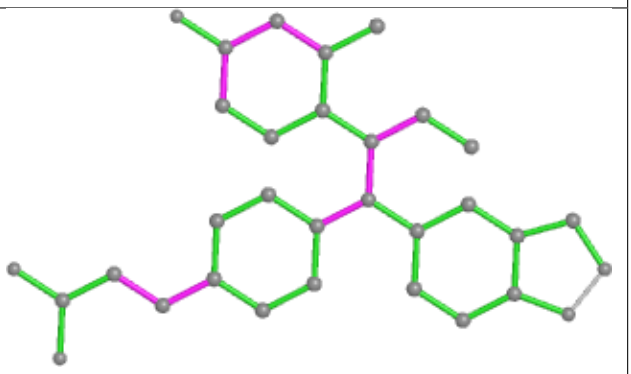
Ligand 7I0 A 601



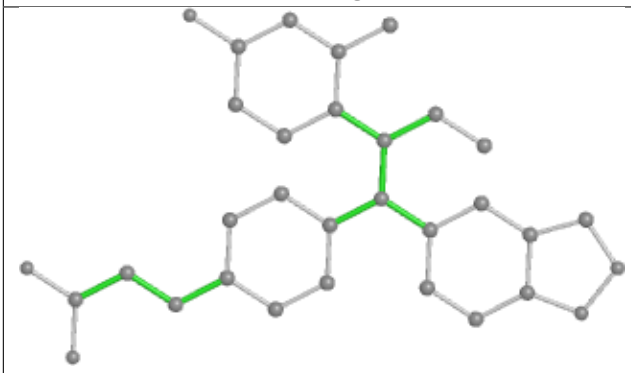
Ligand 7I0 D 602



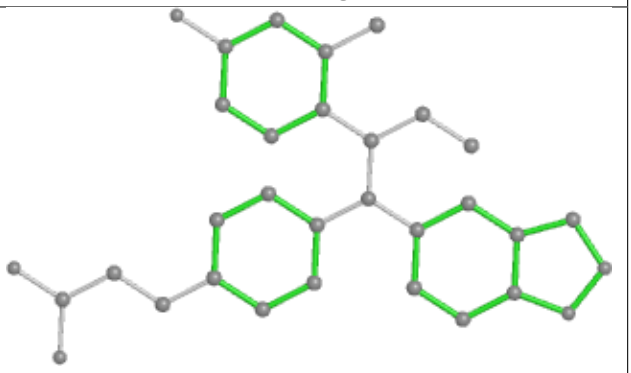
Bond lengths



Bond angles

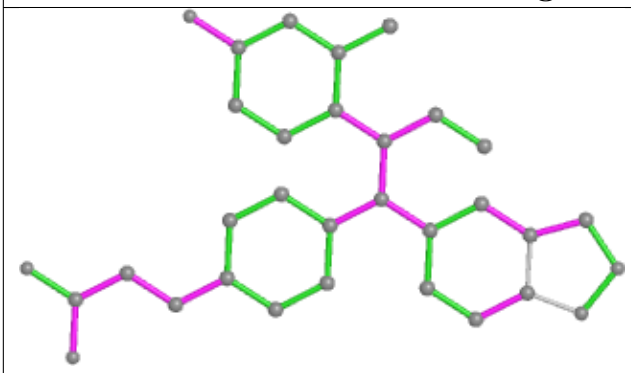


Torsions

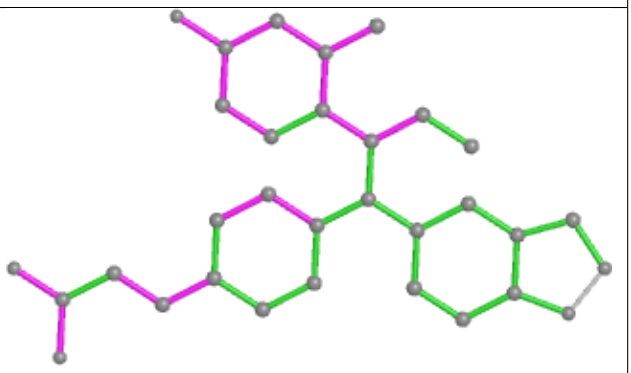


Rings

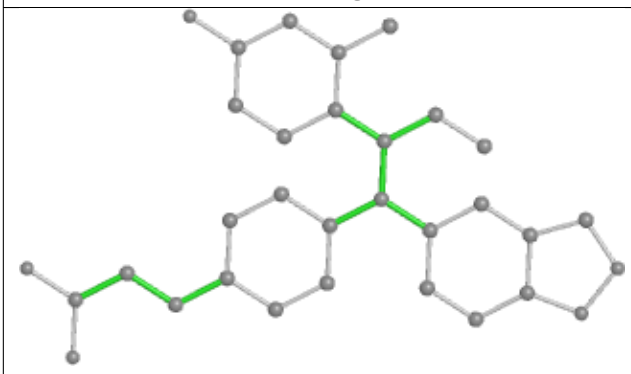
Ligand 7I0 C 601



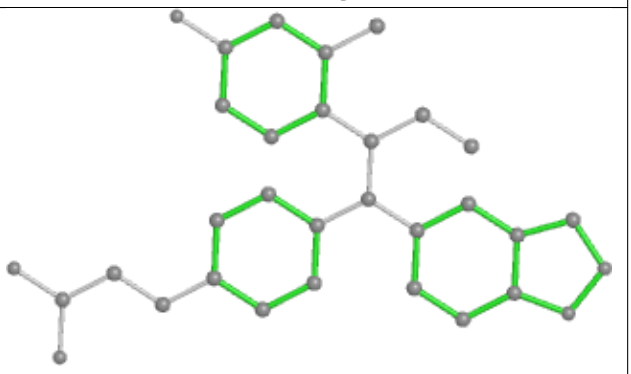
Bond lengths



Bond angles

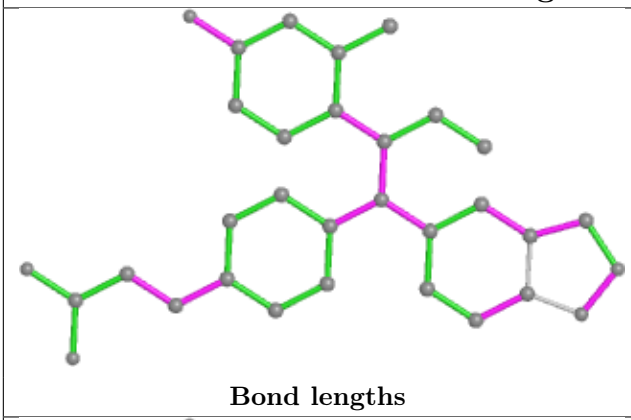


Torsions

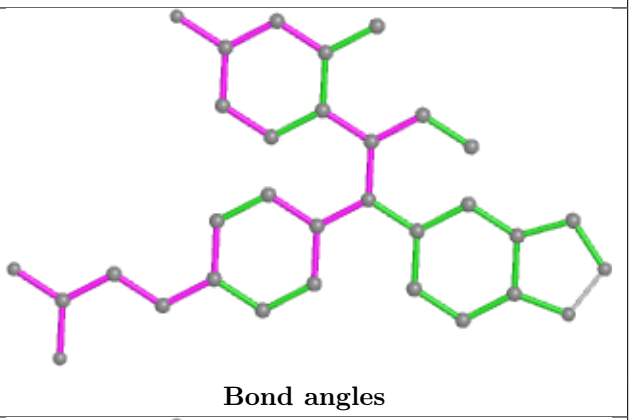


Rings

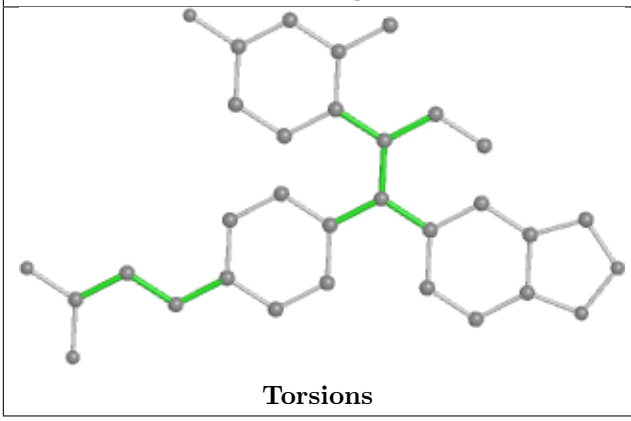
Ligand 7I0 B 602



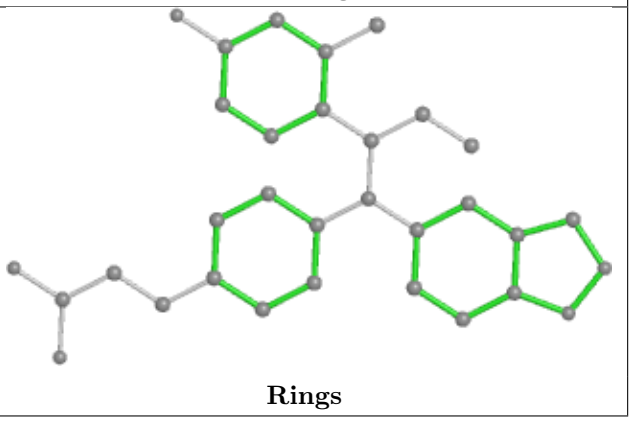
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	243/257 (94%)	0.23	11 (4%)	33	31	18, 31, 60, 96	0
1	B	245/257 (95%)	0.40	18 (7%)	15	14	16, 31, 68, 108	0
1	C	243/257 (94%)	0.17	10 (4%)	37	35	17, 30, 61, 108	0
1	D	242/257 (94%)	0.46	17 (7%)	16	16	17, 32, 76, 123	0
All	All	973/1028 (94%)	0.31	56 (5%)	23	22	16, 31, 69, 123	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	468	SER	9.2
1	D	304	ASN	8.1
1	D	467	LYS	8.1
1	A	462	LEU	7.5
1	C	462	LEU	7.5
1	D	469	LEU	7.3
1	B	304	ASN	7.1
1	D	337	PHE	7.0
1	B	337	PHE	5.8
1	B	418	VAL	5.8
1	B	420	GLY	5.7
1	B	419	GLU	5.6
1	C	530	CYS	5.4
1	B	462	LEU	5.3
1	B	526	TYR	4.3
1	B	464	SER	4.3
1	C	532	ASN	4.3
1	D	340	ALA	4.3
1	A	300	ARG	4.3
1	C	526	TYR	4.2
1	B	463	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	526	TYR	4.0
1	A	461	PHE	4.0
1	B	546	ALA	3.9
1	C	460	THR	3.9
1	B	417	CYS	3.6
1	D	306	LEU	3.4
1	A	331	TYR	3.3
1	B	338	SER	3.3
1	B	547	HIS	3.3
1	B	340	ALA	3.2
1	A	332	ASP	3.1
1	B	303	LYS	3.1
1	D	459	TYR	3.1
1	D	305	SER	3.0
1	D	530	CYS	3.0
1	A	469	LEU	3.0
1	D	552	PRO	2.9
1	A	305	SER	2.9
1	A	301	SER	2.9
1	D	461	PHE	2.8
1	D	334	THR	2.8
1	C	331	TYR	2.8
1	D	331	TYR	2.5
1	B	306	LEU	2.5
1	B	548	ARG	2.4
1	D	529	LYS	2.3
1	D	549	LEU	2.3
1	C	464	SER	2.2
1	A	459	TYR	2.1
1	C	461	PHE	2.1
1	A	466	LEU	2.1
1	D	528	MET	2.1
1	C	469	LEU	2.1
1	C	459	TYR	2.1
1	B	411	ASP	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	YCM	A	381	10/11	0.95	0.10	17,24,50,66	0
1	YCM	C	381	10/11	0.95	0.11	18,31,56,73	0
1	YCM	B	381	10/11	0.96	0.10	19,28,61,66	0
1	YCM	D	381	10/11	0.96	0.12	20,37,77,85	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

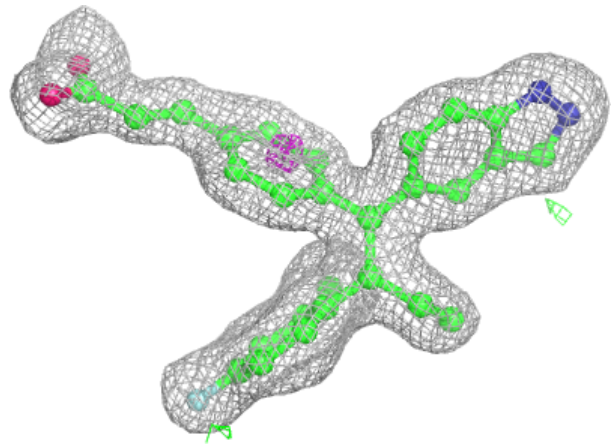
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

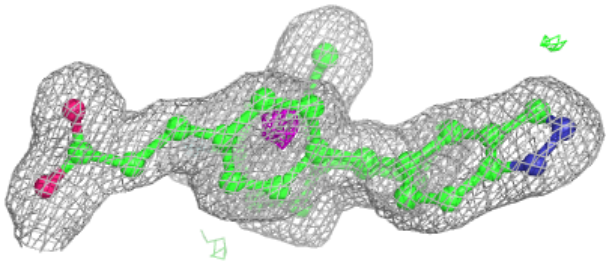
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	7I0	D	602	32/32	0.95	0.09	18,26,36,40	0
2	7I0	B	602	32/32	0.96	0.09	16,25,33,35	0
2	7I0	C	601	32/32	0.96	0.09	16,20,26,30	0
2	7I0	A	601	32/32	0.96	0.07	16,19,27,29	0
3	CL	B	601	1/1	0.99	0.06	36,36,36,36	0
3	CL	D	601	1/1	0.99	0.09	34,34,34,34	0

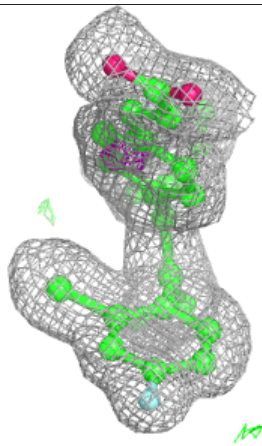
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7I0 D 602:

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

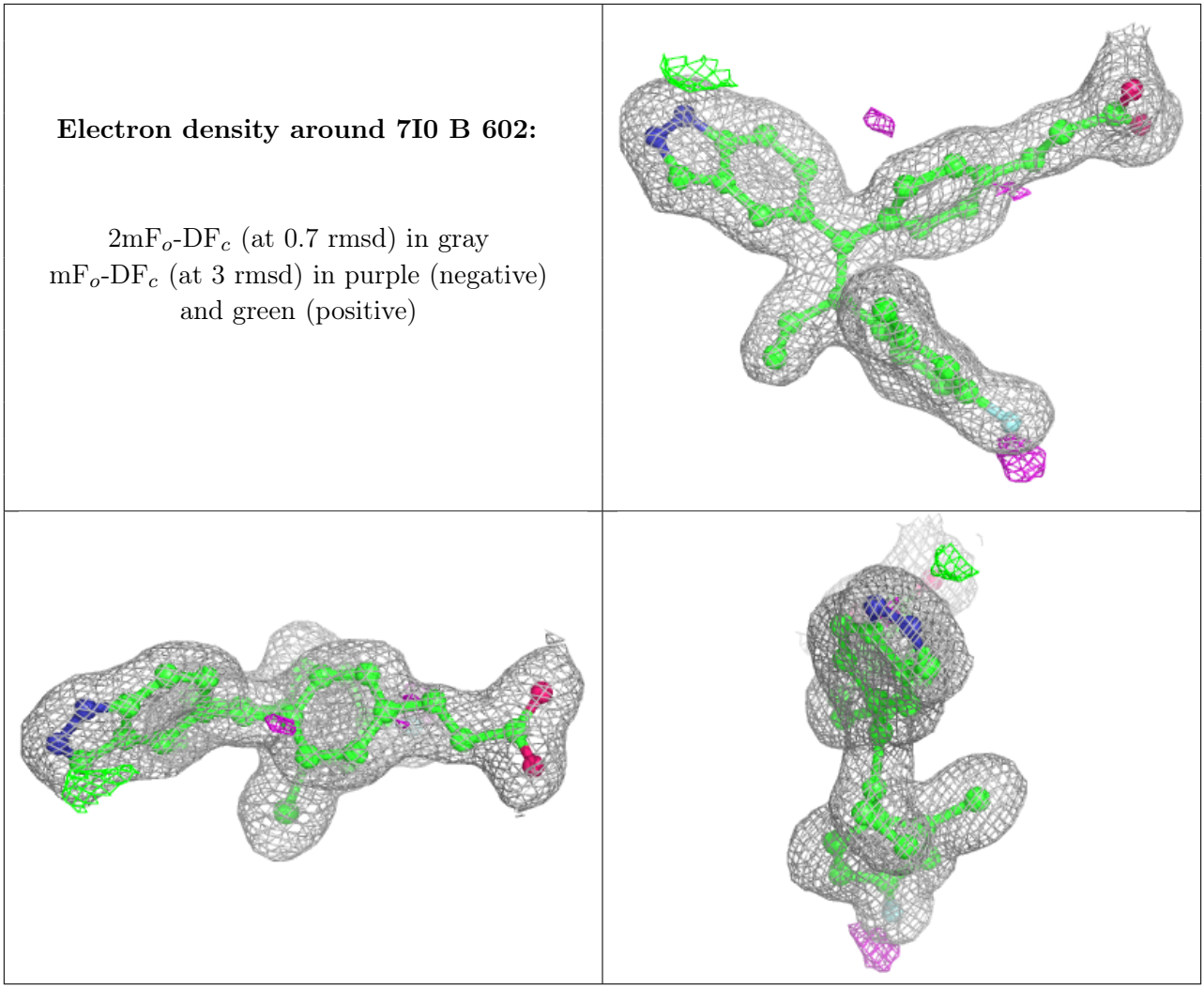






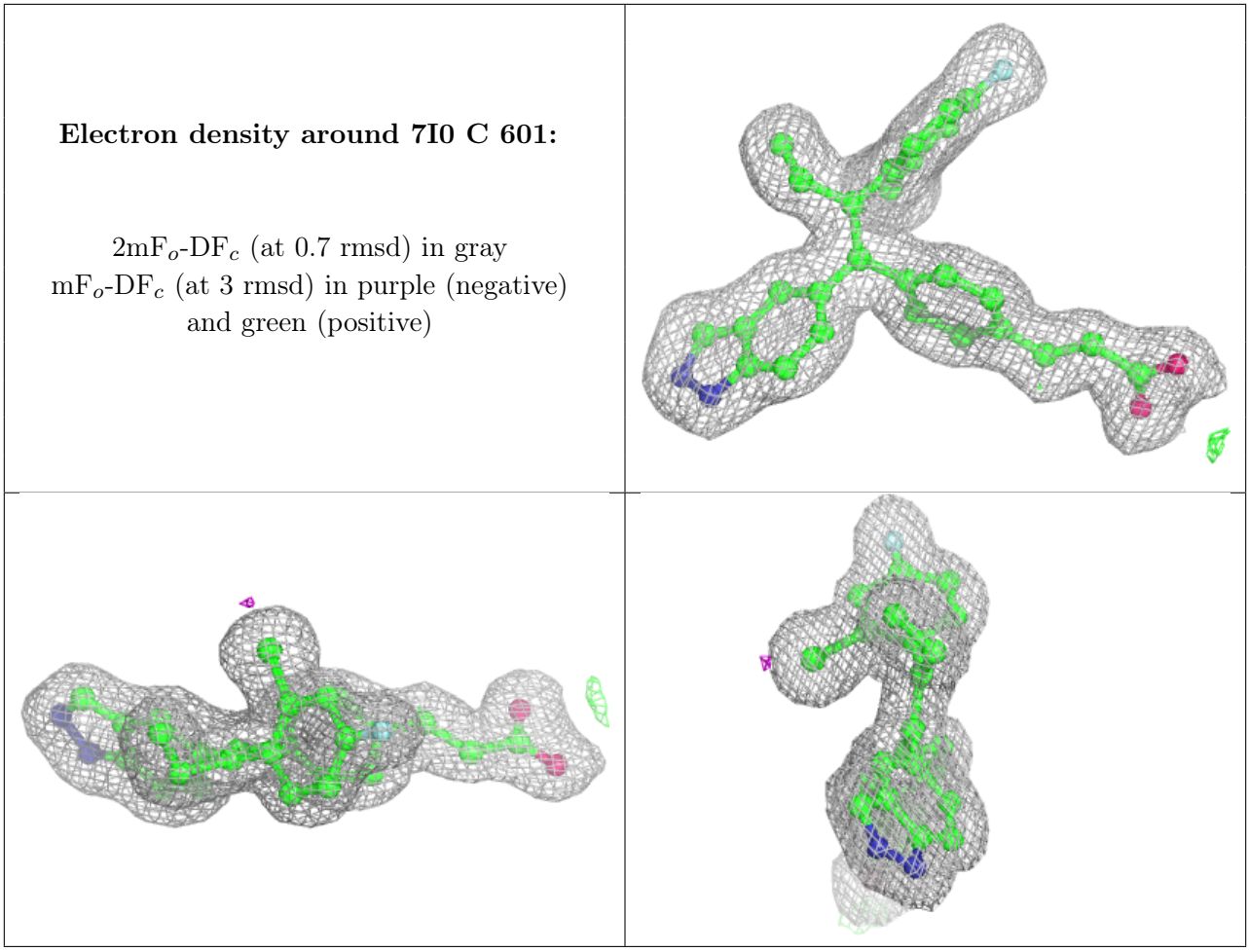
Electron density around 7I0 B 602:

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



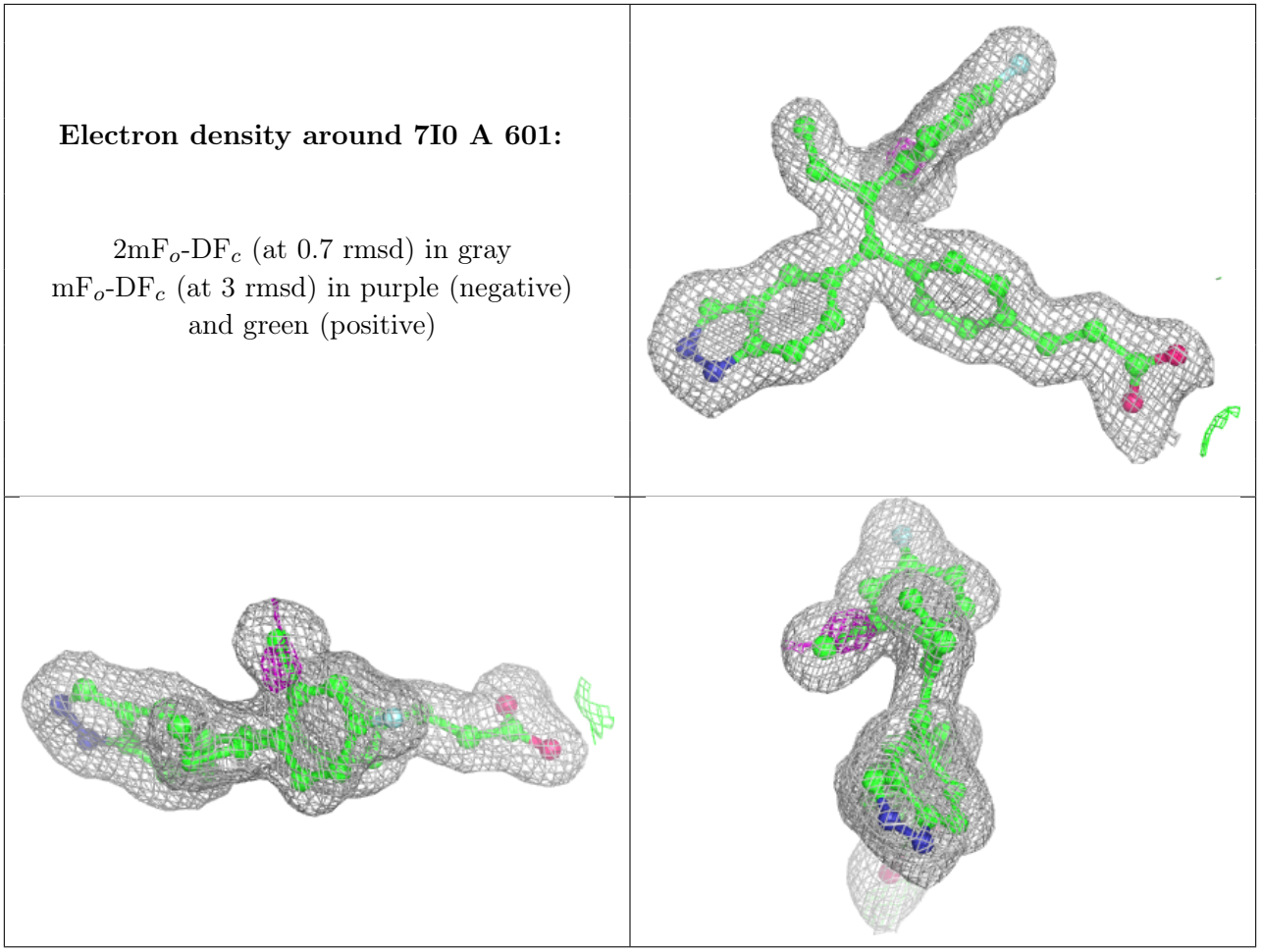
Electron density around 7I0 C 601:

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



Electron density around 7I0 A 601:

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



6.5 Other polymers

There are no such residues in this entry.