Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 12:59 AM EDT

PDB ID	:	7RRZ
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-30
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	:	1.83 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:

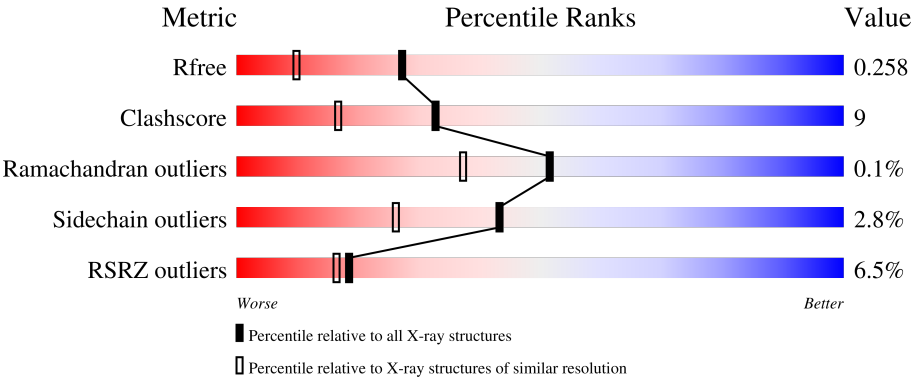
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	9% 75% 16% • 9%
1	B	257	5% 78% 11% 11%
1	C	257	5% 80% 8% • 11%
1	D	257	5% 74% 11% • 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7810 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.

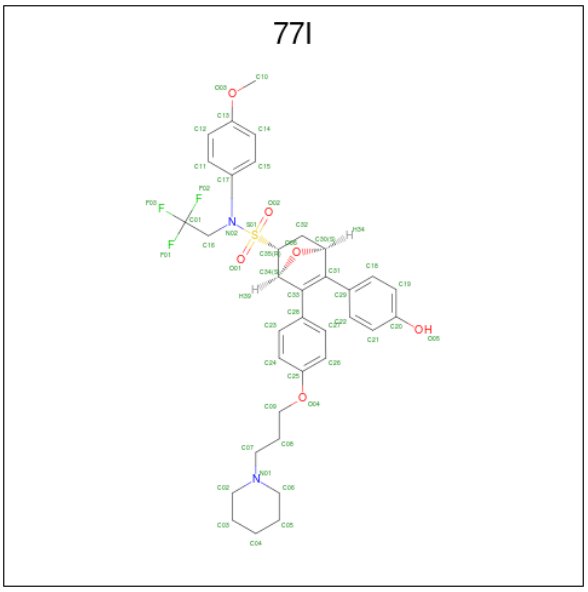
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1870	1198	315	340	17			
1	B	229	Total	C	N	O	S	0	1	0
			1836	1177	311	331	17			
1	C	229	Total	C	N	O	S	0	1	0
			1838	1178	311	334	15			
1	D	218	Total	C	N	O	S	0	1	0
			1755	1127	297	315	16			

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 (1S,2R,4S,5R,6S)-5-(4-hydroxyphenyl)-N-(4-methoxyphenyl)-6-{4-[3-(piperidin-1-yl)propoxy]phenyl}-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]heptane-2-sulfonamide (three-letter code: 77I) (formula: $C_{35}H_{39}F_3N_2O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C F N O S 94 70 6 4 12 2	0	1
2	B	1	Total C F N O S 47 35 3 2 6 1	0	0
2	C	1	Total C N O S 44 35 2 6 1	0	0
2	D	1	Total C F N O S 47 35 3 2 6 1	0	0

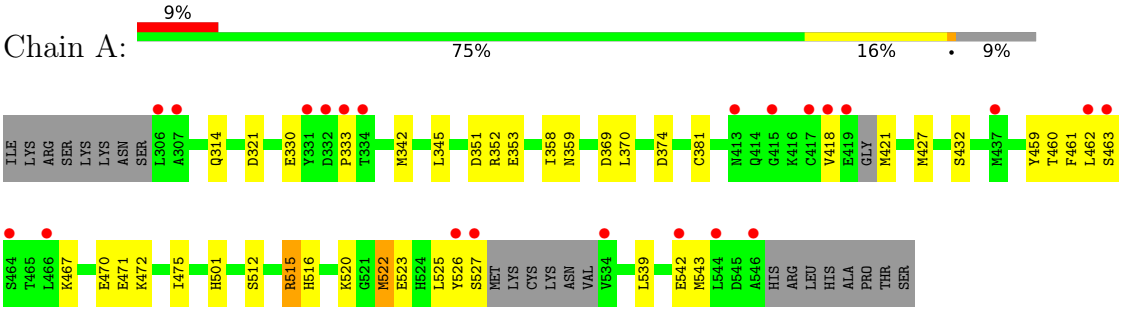
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	0	0
3	B	76	Total O 76 76	0	0
3	C	59	Total O 59 59	0	0
3	D	77	Total O 77 77	0	0

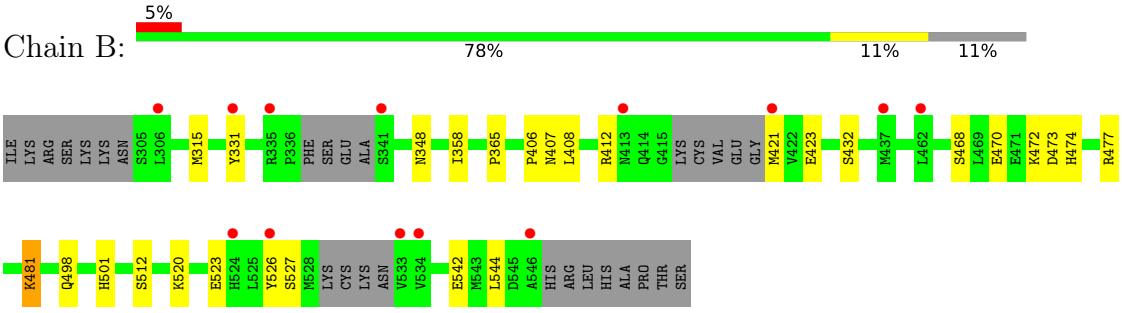
3 Residue-property plots (i)

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.

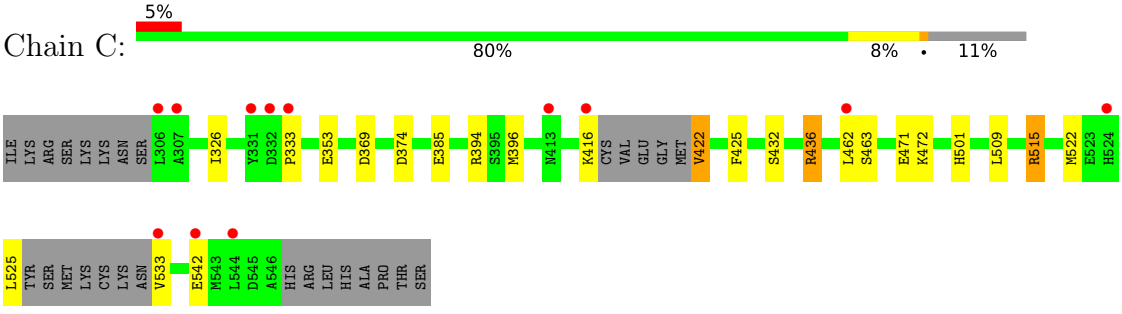
• Molecule 1: Estrogen receptor



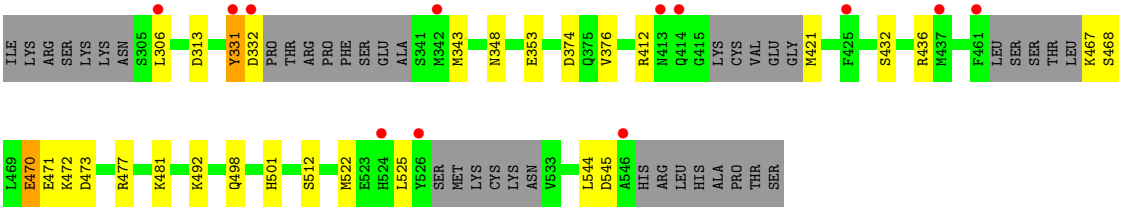
• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor


ILE LYS ARG SER LYS LYS ASN S305 L306 D313 Y331 D332 PRO THR ARG PRO PHE SER GLU ALA S341 M342 M343 N348 E353 D374 Q375 V376 R412 N413 Q414 C415 LYS CYS VAL GLU GLY M421 F425 S432 R436 M437 F461 LEU SER SER THR LEU K467 S468
L469 E470 E471 K472 D473 R477 K481 K492 Q498 H501 S512 M522 E523 H524 L525 Y526 SER MET LYS CYS LYS ASN V533 L544 D545 A546 HIS ARG LEU HIS ALA PRO THR SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.55Å 58.91Å 93.46Å 87.24° 75.18° 62.93°	Depositor
Resolution (Å)	32.86 – 1.83 52.30 – 1.83	Depositor EDS
% Data completeness (in resolution range)	63.4 (32.86-1.83) 63.4 (52.30-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.245 , 0.258 0.245 , 0.258	Depositor DCC
R_{free} test set	2677 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 11.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.109 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7810	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% 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: 77I, 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	0.59	0/1893	0.78	3/2557 (0.1%)
1	B	0.60	0/1861	0.79	0/2513
1	C	0.63	0/1860	0.80	3/2513 (0.1%)
1	D	0.59	0/1777	0.77	2/2396 (0.1%)
All	All	0.60	0/7391	0.78	8/9979 (0.1%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	515	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	C	515	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	A	515	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	C	515	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	C	436	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	D	313	ASP	CB-CG-OD1	5.66	123.39	118.30
1	D	436	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	342	MET	CG-SD-CE	-5.07	92.09	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	526	TYR	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	1870	0	1907	49	0
1	B	1836	0	1878	37	0
1	C	1838	0	1878	22	0
1	D	1755	0	1790	27	0
2	A	94	0	0	7	0
2	B	47	0	0	0	0
2	C	44	0	0	3	0
2	D	47	0	0	2	0
3	A	67	0	0	27	1
3	B	76	0	0	27	1
3	C	59	0	0	9	0
3	D	77	0	0	19	0
All	All	7810	0	7453	130	1

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 9.

All (130) 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:D:477:ARG:HD2	3:D:707:HOH:O	1.32	1.28
1:A:501:HIS:CE1	1:B:501[B]:HIS:CE1	2.27	1.22
1:A:427:MET:SD	3:A:764:HOH:O	1.99	1.16
1:B:407:ASN:CA	3:B:703:HOH:O	1.91	1.16
1:D:343:MET:SD	3:D:777:HOH:O	2.00	1.14
1:D:477:ARG:CD	3:D:707:HOH:O	1.87	1.14
1:A:525:LEU:N	3:A:701:HOH:O	1.87	1.06
1:B:408:LEU:N	3:B:703:HOH:O	1.89	1.06
1:D:472:LYS:N	3:D:701:HOH:O	1.87	1.06
1:D:471:GLU:C	3:D:701:HOH:O	1.95	1.04
1:A:501:HIS:HE1	1:B:501[B]:HIS:CE1	1.68	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:HIS:CE1	1:B:501[B]:HIS:HE1	1.68	1.04
1:B:473:ASP:OD2	1:B:477:ARG:NH1	1.92	1.02
1:D:477:ARG:NE	3:D:702:HOH:O	1.87	1.02
1:B:412:ARG:CZ	3:B:706:HOH:O	2.09	1.00
1:D:473:ASP:N	3:D:701:HOH:O	1.96	0.99
1:A:314:GLN:OE1	3:A:702:HOH:O	1.81	0.98
1:B:412:ARG:NH2	3:B:706:HOH:O	1.95	0.98
1:A:522:MET:O	3:A:701:HOH:O	1.81	0.97
1:B:407:ASN:N	3:B:703:HOH:O	1.93	0.97
1:B:523:GLU:OE1	3:B:701:HOH:O	1.83	0.96
1:A:352:ARG:NH2	3:A:709:HOH:O	1.99	0.95
1:B:407:ASN:C	3:B:703:HOH:O	2.02	0.93
1:D:470:GLU:C	3:D:701:HOH:O	2.07	0.92
1:B:406:PRO:C	3:B:703:HOH:O	2.05	0.92
1:A:321:ASP:OD2	3:A:703:HOH:O	1.88	0.91
1:B:348:ASN:HB3	3:B:704:HOH:O	1.71	0.90
1:A:369:ASP:OD2	3:A:704:HOH:O	1.89	0.89
1:C:422:VAL:HG12	1:C:425:PHE:H	1.38	0.87
1:A:330:GLU:OE2	3:A:706:HOH:O	1.91	0.87
1:A:542:GLU:OE2	3:A:707:HOH:O	1.91	0.87
1:D:470:GLU:O	3:D:701:HOH:O	1.91	0.86
1:A:523:GLU:C	3:A:701:HOH:O	2.15	0.85
1:B:348:ASN:OD1	3:B:704:HOH:O	1.94	0.85
1:D:471:GLU:OE2	3:D:703:HOH:O	1.94	0.84
1:C:369:ASP:OD1	3:C:701:HOH:O	1.95	0.83
1:B:523:GLU:OE2	3:B:705:HOH:O	1.94	0.83
1:C:525:LEU:HD11	1:C:533:VAL:N	1.94	0.82
1:A:359:ASN:OD1	3:A:708:HOH:O	1.98	0.80
1:D:477:ARG:CD	3:D:702:HOH:O	2.27	0.79
1:B:542:GLU:OE1	3:B:707:HOH:O	2.01	0.79
1:C:542:GLU:OE2	3:C:702:HOH:O	2.03	0.76
1:D:477:ARG:HD2	3:D:702:HOH:O	1.87	0.75
1:B:348:ASN:CB	3:B:704:HOH:O	2.32	0.75
1:B:520:LYS:HD2	3:B:701:HOH:O	1.86	0.75
1:A:330:GLU:HG2	3:A:706:HOH:O	1.87	0.73
1:A:543:MET:SD	3:A:715:HOH:O	2.45	0.73
1:B:406:PRO:O	3:B:703:HOH:O	2.04	0.73
1:C:369:ASP:OD2	3:C:701:HOH:O	2.05	0.73
1:B:348:ASN:CG	3:B:704:HOH:O	2.28	0.72
1:A:369:ASP:OD1	3:A:704:HOH:O	2.06	0.72
1:D:348:ASN:OD1	3:D:704:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:LYS:HE2	3:B:708:HOH:O	1.89	0.71
1:C:369:ASP:CG	3:C:701:HOH:O	2.29	0.71
1:A:539:LEU:HG	3:A:715:HOH:O	1.90	0.70
1:A:369:ASP:CG	3:A:704:HOH:O	2.27	0.69
2:A:601[B]:77I:C11	2:A:601[B]:77I:O01	2.41	0.68
1:C:515:ARG:NE	3:C:705:HOH:O	2.26	0.67
1:D:525:LEU:HD12	2:D:601:77I:C13	2.28	0.64
1:A:418:VAL:HB	1:A:421:MET:N	2.15	0.62
1:B:421:MET:SD	3:B:768:HOH:O	2.56	0.61
1:A:501:HIS:CE1	1:B:501[B]:HIS:ND1	2.68	0.61
1:A:501:HIS:ND1	1:B:501[B]:HIS:CE1	2.67	0.61
1:A:459:TYR:C	3:A:705:HOH:O	2.39	0.60
1:D:473:ASP:OD2	3:D:702:HOH:O	2.16	0.60
1:D:492:LYS:HD2	3:D:722:HOH:O	2.02	0.59
1:A:520:LYS:NZ	3:A:716:HOH:O	2.35	0.59
1:A:381:YCM:OZ1	3:A:711:HOH:O	2.17	0.59
1:D:471:GLU:N	3:D:701:HOH:O	2.34	0.59
1:B:472:LYS:CE	3:B:708:HOH:O	2.50	0.58
1:A:418:VAL:CG2	1:A:421:MET:N	2.67	0.57
1:C:515:ARG:HD2	3:C:705:HOH:O	2.05	0.57
1:A:460:THR:N	3:A:705:HOH:O	2.36	0.57
1:C:422:VAL:HG12	1:C:425:PHE:HB2	1.87	0.56
1:C:515:ARG:CD	3:C:705:HOH:O	2.53	0.56
1:A:516:HIS:CD2	3:A:764:HOH:O	2.59	0.56
1:A:351:ASP:OD1	2:A:601[A]:77I:N01	2.40	0.55
1:A:330:GLU:CG	3:A:706:HOH:O	2.51	0.54
1:C:525:LEU:HD12	2:C:601:77I:C13	2.38	0.54
1:B:520:LYS:CE	3:B:701:HOH:O	2.56	0.54
1:A:330:GLU:CD	3:A:706:HOH:O	2.43	0.51
1:A:501:HIS:ND1	1:B:501[B]:HIS:ND1	2.58	0.51
1:B:407:ASN:HA	3:B:703:HOH:O	1.84	0.51
1:C:463:SER:OG	1:C:472:LYS:NZ	2.44	0.51
1:C:353:GLU:OE1	2:C:601:77I:O05	2.30	0.50
1:C:396:MET:O	1:C:436:ARG:HD3	2.12	0.50
1:D:331:TYR:O	1:D:332:ASP:C	2.50	0.50
1:C:333:PRO:CD	3:C:755:HOH:O	2.60	0.50
1:A:463:SER:OG	1:A:472:LYS:NZ	2.44	0.50
1:B:315:MET:CE	1:B:481:LYS:HG2	2.42	0.49
1:B:520:LYS:HE3	3:B:701:HOH:O	2.12	0.49
1:A:358:ILE:HG12	1:A:543:MET:HE2	1.93	0.49
1:B:421:MET:CE	3:B:768:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:GLU:OE1	2:D:601:77I:O05	2.31	0.48
1:C:416:LYS:HD2	1:C:422:VAL:HG23	1.94	0.48
1:C:385:GLU:OE2	3:C:705:HOH:O	2.20	0.47
1:D:477:ARG:HG2	1:D:477:ARG:HH11	1.80	0.47
1:C:525:LEU:HD12	2:C:601:77I:O03	2.14	0.47
1:A:353:GLU:OE1	2:A:601[A]:77I:O05	2.33	0.47
1:A:526:TYR:HA	3:A:719:HOH:O	2.15	0.46
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.98	0.46
1:A:467:LYS:HA	1:A:470:GLU:HG2	1.97	0.46
1:B:365:PRO:HA	3:B:725:HOH:O	2.15	0.46
1:B:421:MET:HG3	1:B:423:GLU:H	1.81	0.45
1:B:474:HIS:ND1	3:B:702:HOH:O	1.83	0.45
1:A:421:MET:HG3	2:A:601[A]:77I:C15	2.47	0.45
1:B:470:GLU:HG2	3:B:712:HOH:O	2.17	0.45
1:A:525:LEU:HD23	1:A:527:SER:H	1.82	0.44
1:C:501:HIS:HB2	3:D:746:HOH:O	2.17	0.44
1:A:461:PHE:N	3:A:705:HOH:O	1.89	0.44
1:D:467:LYS:HG3	1:D:468:SER:N	2.32	0.44
1:A:516:HIS:HD2	3:A:764:HOH:O	1.96	0.44
1:B:468:SER:OG	3:B:708:HOH:O	2.21	0.44
1:A:418:VAL:CB	1:A:421:MET:N	2.81	0.44
1:A:421:MET:HG3	2:A:601[A]:77I:C17	2.48	0.44
1:D:348:ASN:HB3	3:D:704:HOH:O	2.19	0.43
1:A:374:ASP:OD2	1:A:471:GLU:OE1	2.37	0.43
1:A:353:GLU:OE1	2:A:601[B]:77I:O05	2.36	0.43
1:D:376:VAL:CG2	1:D:544:LEU:HD12	2.50	0.42
1:D:481:LYS:HE3	1:D:481:LYS:HB3	1.93	0.42
1:D:477:ARG:NE	3:D:707:HOH:O	2.32	0.41
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.38	0.41
1:B:498:GLN:HA	1:B:501[A]:HIS:CE1	2.55	0.41
1:C:509:LEU:HD23	1:C:509:LEU:HA	1.90	0.41
1:D:374:ASP:OD2	1:D:471:GLU:OE1	2.38	0.40
1:C:326:ILE:HD12	1:C:394:ARG:HD3	2.01	0.40
1:A:351:ASP:OD1	2:A:601[B]:77I:N01	2.55	0.40
1:A:333:PRO:HB3	1:A:345:LEU:HD21	2.03	0.40
1:A:515:ARG:NE	3:A:722:HOH:O	2.53	0.40
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.56	0.40

All (1) 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)
3:A:706:HOH:O	3:B:716:HOH:O[1_645]	2.09	0.11

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	227/257 (88%)	221 (97%)	6 (3%)	0	100 100
1	B	221/257 (86%)	216 (98%)	5 (2%)	0	100 100
1	C	223/257 (87%)	220 (99%)	3 (1%)	0	100 100
1	D	208/257 (81%)	202 (97%)	5 (2%)	1 (0%)	29 15
All	All	879/1028 (86%)	859 (98%)	19 (2%)	1 (0%)	51 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	545	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	210/231 (91%)	206 (98%)	4 (2%)	57 42
1	B	207/231 (90%)	200 (97%)	7 (3%)	37 19
1	C	206/231 (89%)	202 (98%)	4 (2%)	57 42
1	D	196/231 (85%)	188 (96%)	8 (4%)	30 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	819/924 (89%)	796 (97%)	23 (3%)	43 26

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	432	SER
1	A	462	LEU
1	A	512	SER
1	A	522	MET
1	B	331	TYR
1	B	358	ILE
1	B	432	SER
1	B	481	LYS
1	B	512	SER
1	B	527	SER
1	B	544	LEU
1	C	422	VAL
1	C	432	SER
1	C	462	LEU
1	C	522	MET
1	D	306	LEU
1	D	331	TYR
1	D	412	ARG
1	D	421	MET
1	D	432	SER
1	D	470	GLU
1	D	512	SER
1	D	522	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	501	HIS
1	A	516	HIS
1	A	519	ASN
1	B	519	ASN
1	C	441	GLN
1	C	513	HIS
1	C	519	ASN
1	C	524	HIS
1	D	413	ASN

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Mol	Chain	Res	Type
1	D	513	HIS
1	D	519	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	D	381	1	7,9,10	0.57	0	4,10,12	0.19	0
1	YCM	C	381	1	7,9,10	0.41	0	4,10,12	0.50	0
1	YCM	A	381	1	7,9,10	0.51	0	4,10,12	0.45	0
1	YCM	B	381	1	7,9,10	0.60	0	4,10,12	0.28	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	D	381	1	-	1/6/8/10	-
1	YCM	C	381	1	-	2/6/8/10	-
1	YCM	A	381	1	-	2/6/8/10	-
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 (6) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	381	YCM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	77I	C	601	-	47,49,52	2.46	5 (10%)	56,70,76	2.87	6 (10%)
2	77I	A	601[B]	-	49,52,52	2.52	5 (10%)	63,76,76	2.08	8 (12%)
2	77I	A	601[A]	-	49,52,52	2.52	5 (10%)	63,76,76	1.61	7 (11%)
2	77I	D	601	-	49,52,52	2.38	5 (10%)	63,76,76	2.78	10 (15%)
2	77I	B	601	-	49,52,52	2.34	5 (10%)	63,76,76	2.41	9 (14%)

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	77I	C	601	-	-	8/33/67/70	0/7/6/6
2	77I	A	601[B]	-	-	9/36/70/70	0/7/6/6
2	77I	A	601[A]	-	-	6/36/70/70	0/7/6/6
2	77I	D	601	-	-	8/36/70/70	0/7/6/6
2	77I	B	601	-	-	18/36/70/70	0/7/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[B]	77I	C17-N02	-13.09	1.26	1.44
2	A	601[A]	77I	C17-N02	-13.07	1.26	1.44
2	C	601	77I	C17-N02	-12.00	1.28	1.44
2	D	601	77I	C17-N02	-11.48	1.28	1.44
2	B	601	77I	C17-N02	-11.35	1.28	1.44
2	B	601	77I	C28-C33	-7.42	1.34	1.48
2	A	601[B]	77I	C29-C31	-7.37	1.34	1.48
2	A	601[A]	77I	C29-C31	-7.31	1.34	1.48
2	C	601	77I	C28-C33	-7.20	1.34	1.48
2	C	601	77I	C29-C31	-6.99	1.35	1.48
2	A	601[B]	77I	C28-C33	-6.99	1.35	1.48
2	D	601	77I	C28-C33	-6.93	1.35	1.48
2	A	601[A]	77I	C28-C33	-6.91	1.35	1.48
2	D	601	77I	C29-C31	-6.82	1.35	1.48
2	B	601	77I	C29-C31	-6.22	1.36	1.48
2	D	601	77I	O01-S01	3.60	1.46	1.43
2	C	601	77I	O02-S01	3.54	1.46	1.43
2	A	601[B]	77I	O02-S01	3.10	1.46	1.43
2	A	601[A]	77I	O01-S01	2.68	1.45	1.43
2	B	601	77I	O02-S01	2.33	1.45	1.43
2	D	601	77I	O02-S01	2.32	1.45	1.43
2	A	601[B]	77I	C16-C01	2.15	1.53	1.50
2	A	601[A]	77I	O02-S01	2.10	1.45	1.43
2	C	601	77I	O06-C34	2.06	1.46	1.43
2	B	601	77I	S01-N02	2.06	1.71	1.67

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	77I	O02-S01-O01	-19.44	106.72	119.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	77I	O02-S01-O01	-18.60	107.27	119.22
2	B	601	77I	O02-S01-O01	-15.53	109.24	119.22
2	A	601[B]	77I	O02-S01-O01	-12.67	111.08	119.22
2	A	601[A]	77I	O02-S01-O01	-9.31	113.24	119.22
2	D	601	77I	O01-S01-N02	5.09	113.78	107.56
2	A	601[B]	77I	O02-S01-N02	4.95	113.62	107.56
2	D	601	77I	C16-N02-C17	4.79	123.98	117.59
2	A	601[B]	77I	C16-N02-C17	4.51	123.62	117.59
2	C	601	77I	O01-S01-N02	4.36	112.89	107.56
2	B	601	77I	O02-S01-N02	4.34	112.87	107.56
2	B	601	77I	C01-C16-N02	-3.98	108.28	112.14
2	B	601	77I	O01-S01-N02	3.94	112.38	107.56
2	A	601[A]	77I	C01-C16-N02	3.87	115.90	112.14
2	B	601	77I	O06-C30-C32	-3.69	97.38	104.64
2	A	601[B]	77I	O06-C30-C32	-3.39	97.96	104.64
2	B	601	77I	F02-C01-C16	-3.39	106.57	112.13
2	D	601	77I	O02-S01-N02	3.33	111.63	107.56
2	D	601	77I	C03-C02-N01	-3.20	106.19	111.33
2	A	601[B]	77I	C10-O03-C13	-3.18	110.61	117.51
2	D	601	77I	O06-C30-C32	-3.14	98.46	104.64
2	A	601[A]	77I	C10-O03-C13	-2.85	111.33	117.51
2	B	601	77I	C23-C28-C33	-2.80	117.28	120.91
2	C	601	77I	O02-S01-N02	2.71	110.88	107.56
2	D	601	77I	C23-C28-C33	-2.70	117.42	120.91
2	C	601	77I	O06-C30-C32	-2.69	99.34	104.64
2	B	601	77I	C16-N02-C17	2.58	121.03	117.59
2	C	601	77I	C07-N01-C06	2.57	117.81	111.23
2	D	601	77I	C06-N01-C02	2.56	114.59	108.83
2	A	601[A]	77I	C16-N02-C17	2.47	120.89	117.59
2	C	601	77I	C27-C28-C33	-2.43	117.76	120.91
2	A	601[A]	77I	F03-C01-C16	-2.38	108.22	112.13
2	A	601[B]	77I	C09-O04-C25	-2.35	111.79	117.93
2	A	601[A]	77I	C11-C17-N02	-2.21	116.86	120.16
2	A	601[A]	77I	O06-C30-C32	-2.19	100.33	104.64
2	A	601[B]	77I	F02-C01-C16	-2.17	108.57	112.13
2	B	601	77I	C07-N01-C02	2.12	116.66	111.23
2	D	601	77I	F03-C01-C16	-2.08	108.72	112.13
2	D	601	77I	C22-C29-C31	-2.07	118.22	120.91
2	A	601[B]	77I	C22-C29-C31	-2.03	118.28	120.91

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601[A]	77I	C34-C35-S01-O02
2	A	601[A]	77I	C16-N02-S01-O01
2	A	601[B]	77I	C17-N02-S01-O01
2	A	601[B]	77I	C16-N02-S01-O01
2	A	601[B]	77I	C16-N02-S01-O02
2	B	601	77I	F02-C01-C16-N02
2	B	601	77I	C17-N02-S01-O01
2	B	601	77I	C16-N02-S01-O01
2	B	601	77I	C16-N02-S01-O02
2	C	601	77I	C17-N02-S01-C35
2	C	601	77I	C17-N02-S01-O01
2	C	601	77I	C16-N02-S01-O01
2	D	601	77I	C17-N02-S01-O01
2	D	601	77I	C16-N02-S01-O01
2	D	601	77I	C16-N02-S01-O02
2	A	601[A]	77I	C07-C08-C09-O04
2	B	601	77I	C08-C07-N01-C02
2	A	601[A]	77I	C08-C07-N01-C06
2	A	601[B]	77I	C08-C07-N01-C02
2	C	601	77I	C08-C07-N01-C06
2	C	601	77I	C07-C08-C09-O04
2	B	601	77I	N01-C07-C08-C09
2	A	601[B]	77I	C15-C17-N02-S01
2	A	601[B]	77I	C11-C17-N02-S01
2	B	601	77I	C11-C17-N02-S01
2	D	601	77I	C11-C17-N02-S01
2	B	601	77I	C12-C13-O03-C10
2	B	601	77I	C14-C13-O03-C10
2	A	601[B]	77I	C08-C07-N01-C06
2	C	601	77I	C08-C07-N01-C02
2	A	601[A]	77I	C08-C07-N01-C02
2	D	601	77I	C08-C07-N01-C06
2	B	601	77I	C08-C09-O04-C25
2	B	601	77I	C24-C25-O04-C09
2	B	601	77I	C26-C25-O04-C09
2	B	601	77I	F03-C01-C16-N02
2	B	601	77I	C16-N02-S01-C35
2	D	601	77I	C16-N02-S01-C35
2	B	601	77I	C07-C08-C09-O04
2	C	601	77I	C15-C17-N02-S01
2	A	601[B]	77I	C16-N02-S01-C35
2	A	601[B]	77I	N01-C07-C08-C09
2	B	601	77I	F01-C01-C16-N02

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Mol	Chain	Res	Type	Atoms
2	C	601	77I	C16-N02-S01-C35
2	B	601	77I	C17-N02-S01-C35
2	B	601	77I	C15-C17-N02-S01
2	D	601	77I	C15-C17-N02-S01
2	D	601	77I	C17-N02-S01-C35
2	A	601[A]	77I	C16-N02-S01-C35

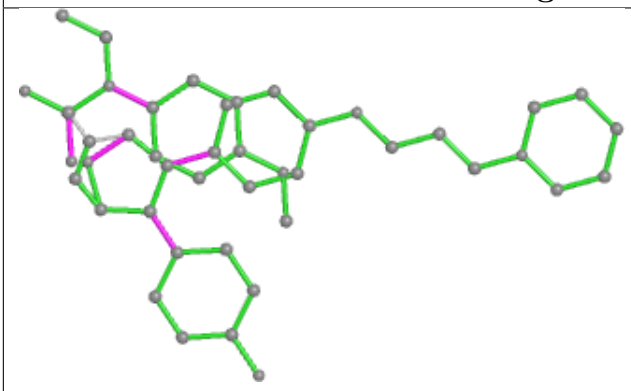
There are no ring outliers.

4 monomers are involved in 12 short contacts:

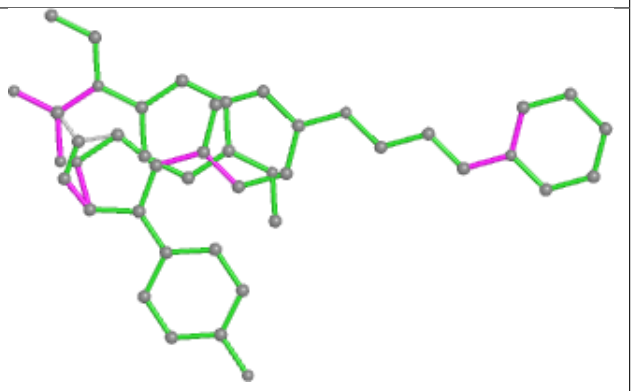
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	77I	3	0
2	A	601[B]	77I	3	0
2	A	601[A]	77I	4	0
2	D	601	77I	2	0

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.

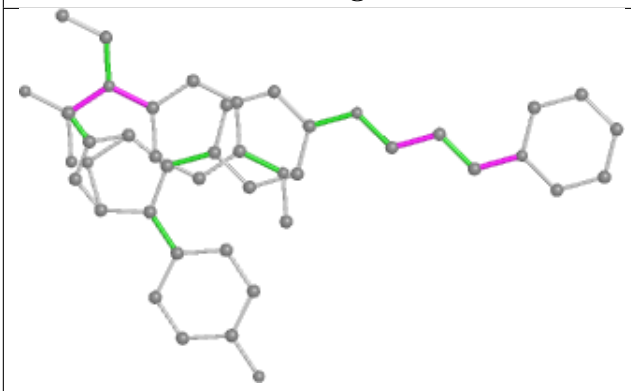
Ligand 77I C 601



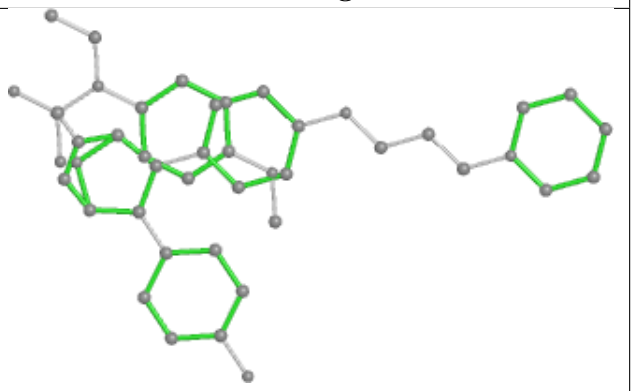
Bond lengths



Bond angles

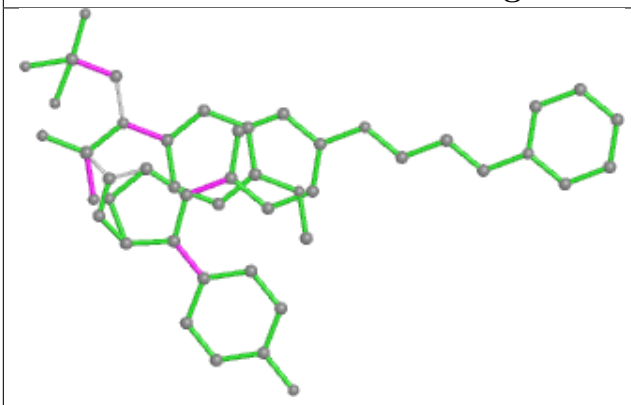


Torsions

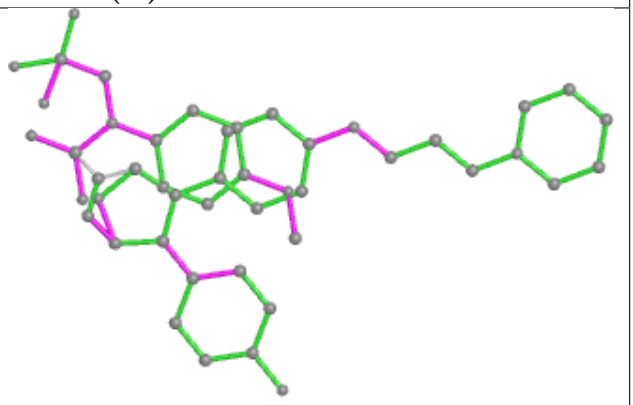


Rings

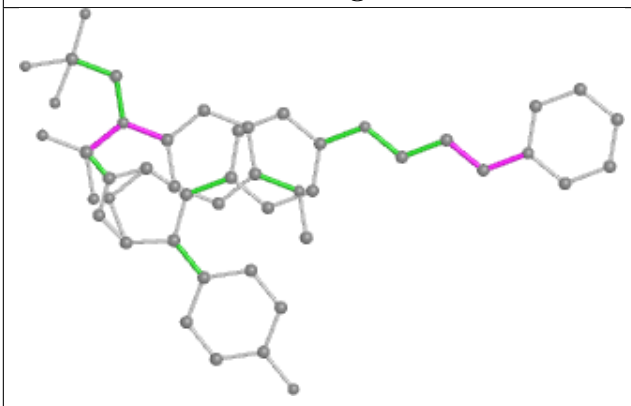
Ligand 77I A 601 (B)



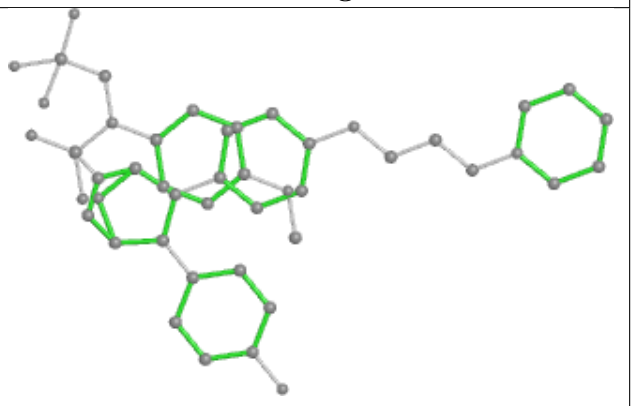
Bond lengths



Bond angles

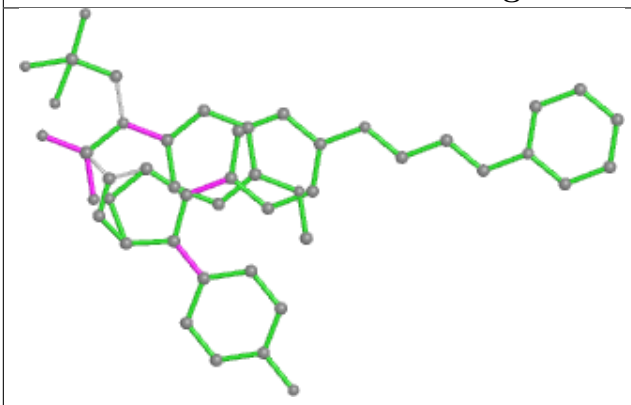


Torsions

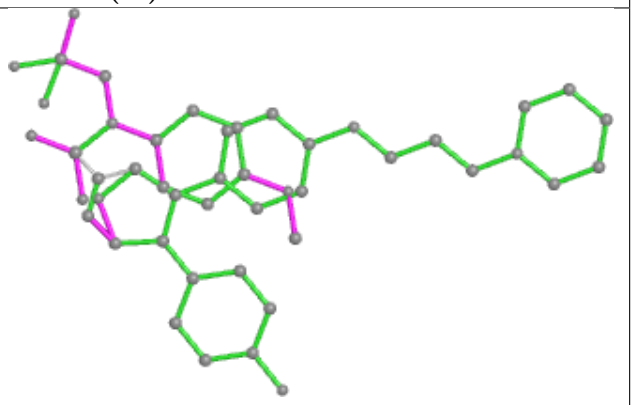


Rings

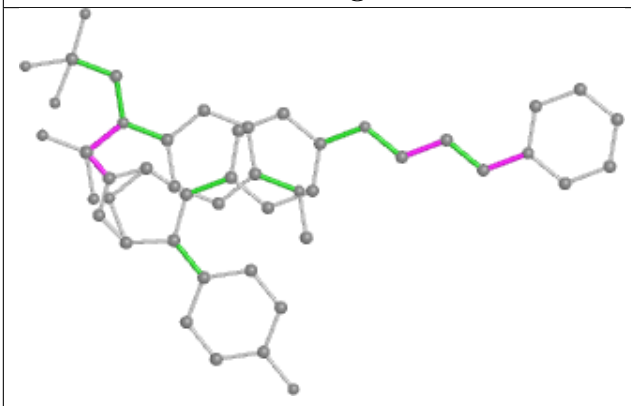
Ligand 77I A 601 (A)



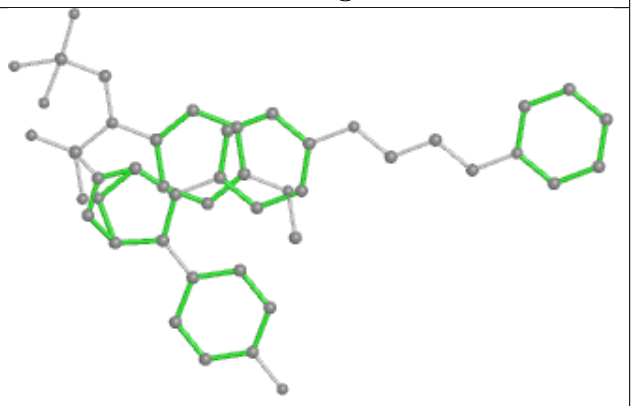
Bond lengths



Bond angles

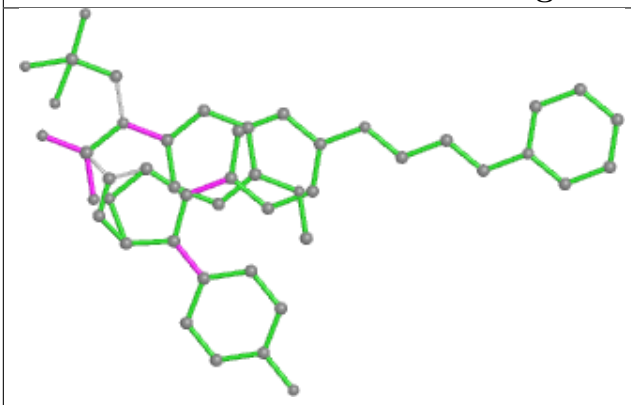


Torsions

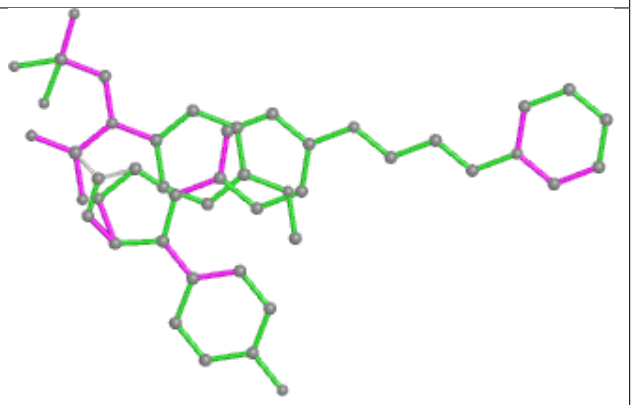


Rings

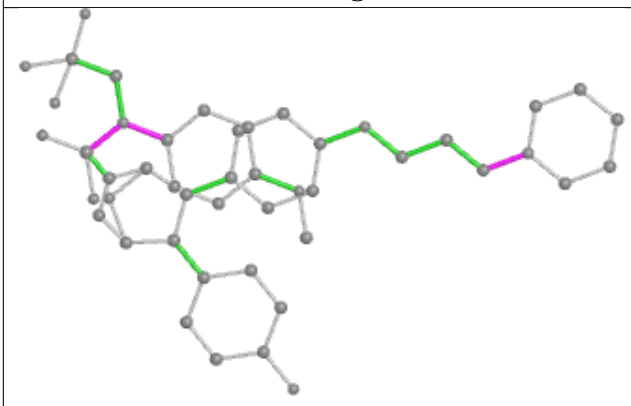
Ligand 77I D 601



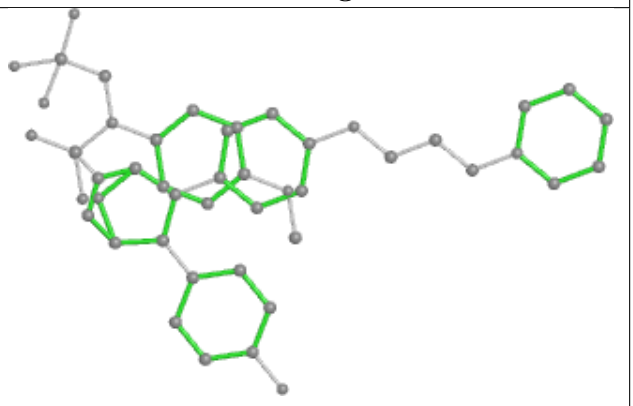
Bond lengths



Bond angles

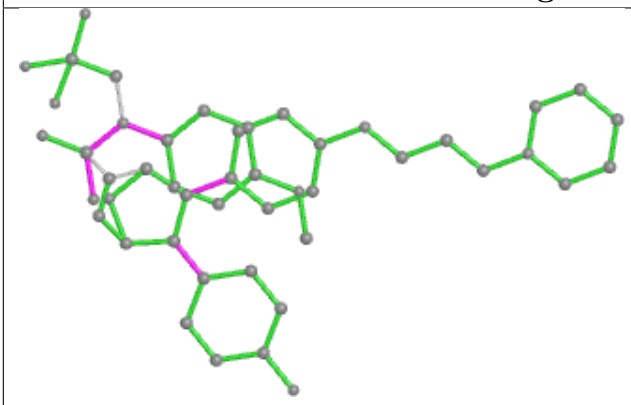


Torsions

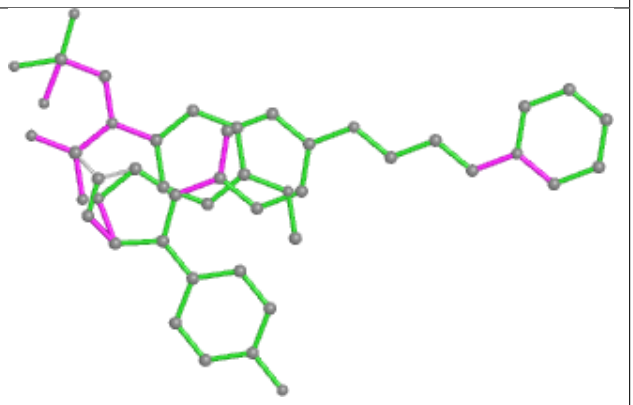


Rings

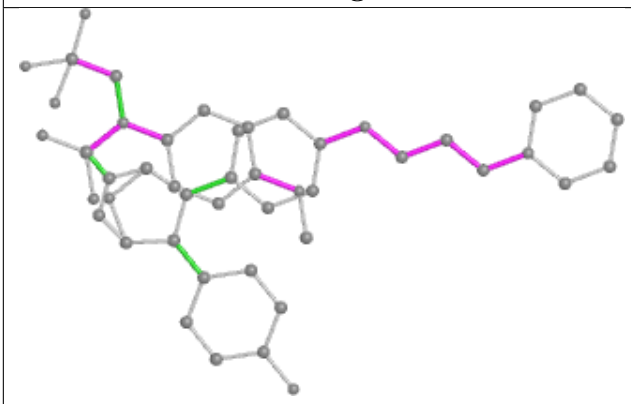
Ligand 77I B 601



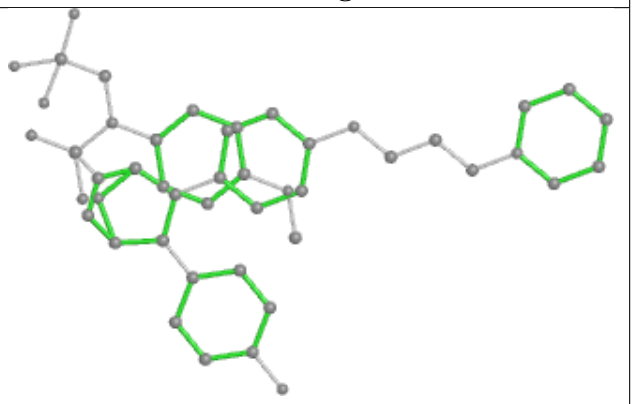
Bond lengths



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	233/257 (90%)	0.48	22 (9%)	8	7	8, 15, 37, 52	0
1	B	228/257 (88%)	0.35	13 (5%)	23	21	8, 13, 36, 49	0
1	C	228/257 (88%)	0.48	12 (5%)	26	24	9, 15, 35, 49	0
1	D	217/257 (84%)	0.39	12 (5%)	25	22	9, 14, 34, 52	0
All	All	906/1028 (88%)	0.43	59 (6%)	18	16	8, 14, 36, 52	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	GLU	7.4
1	A	418	VAL	7.2
1	A	462	LEU	6.6
1	A	526	TYR	5.1
1	B	331	TYR	4.9
1	B	526	TYR	4.6
1	D	526	TYR	4.6
1	C	416	LYS	4.4
1	C	462	LEU	4.2
1	C	413	ASN	4.1
1	D	332	ASP	4.1
1	A	307	ALA	4.1
1	D	331	TYR	3.9
1	D	546	ALA	3.8
1	A	464	SER	3.8
1	A	463	SER	3.8
1	D	413	ASN	3.7
1	A	334	THR	3.7
1	D	461	PHE	3.7
1	B	306	LEU	3.4
1	B	533	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	335	ARG	3.3
1	B	524	HIS	3.2
1	D	524	HIS	3.2
1	A	306	LEU	3.2
1	B	462	LEU	3.2
1	A	544	LEU	3.0
1	A	332	ASP	3.0
1	D	306	LEU	2.9
1	A	331	TYR	2.9
1	C	306	LEU	2.9
1	C	331	TYR	2.9
1	A	417	CYS	2.9
1	B	437	MET	2.9
1	A	546	ALA	2.7
1	D	342	MET	2.7
1	C	542	GLU	2.6
1	B	413	ASN	2.6
1	C	307	ALA	2.5
1	A	466	LEU	2.5
1	D	414	GLN	2.5
1	B	421	MET	2.5
1	A	534	VAL	2.4
1	C	544	LEU	2.4
1	C	524	HIS	2.4
1	C	533	VAL	2.4
1	D	437	MET	2.3
1	D	425	PHE	2.3
1	C	332	ASP	2.3
1	B	341	SER	2.3
1	A	527	SER	2.3
1	A	333	PRO	2.3
1	A	437	MET	2.2
1	B	546	ALA	2.2
1	A	542	GLU	2.2
1	A	415	GLY	2.1
1	A	413	ASN	2.1
1	C	333	PRO	2.1
1	B	534	VAL	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	C	381	10/11	0.87	0.17	12,14,23,24	0
1	YCM	B	381	10/11	0.89	0.17	11,13,20,20	0
1	YCM	A	381	10/11	0.91	0.14	12,14,22,24	0
1	YCM	D	381	10/11	0.91	0.12	12,14,20,22	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

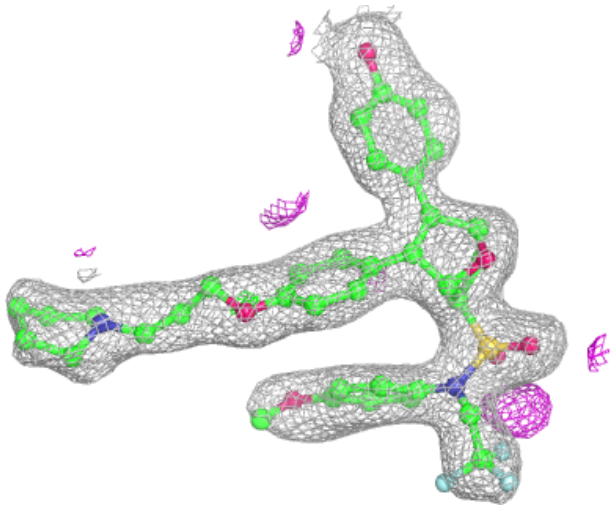
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

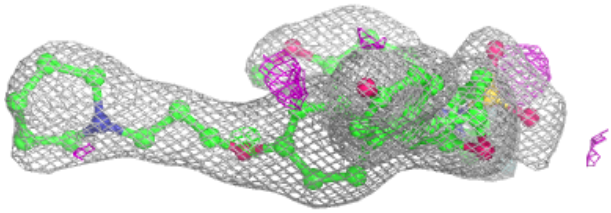
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	77I	B	601	47/47	0.90	0.16	26,32,48,55	0
2	77I	D	601	47/47	0.90	0.17	28,36,53,58	0
2	77I	A	601[A]	47/47	0.91	0.19	27,31,37,40	47
2	77I	C	601	44/47	0.91	0.17	21,32,46,48	0
2	77I	A	601[B]	47/47	0.91	0.19	26,31,37,39	47

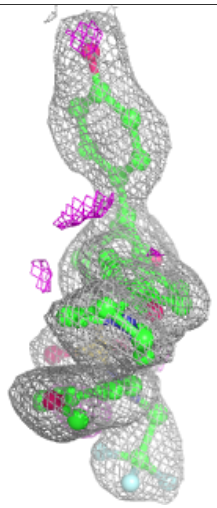
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 77I B 601:

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

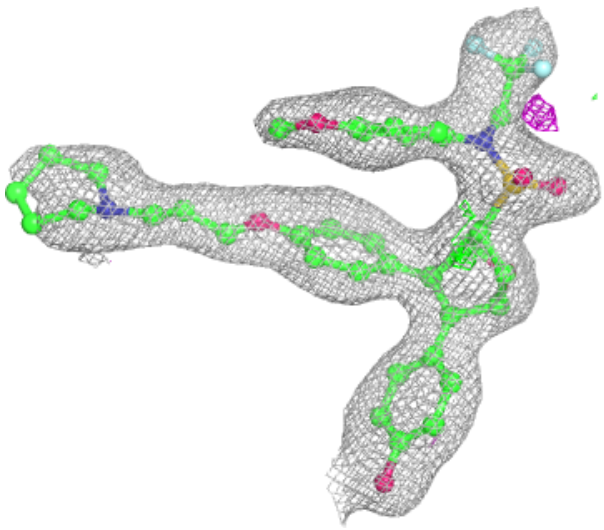


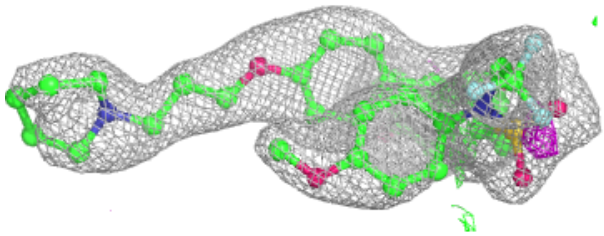


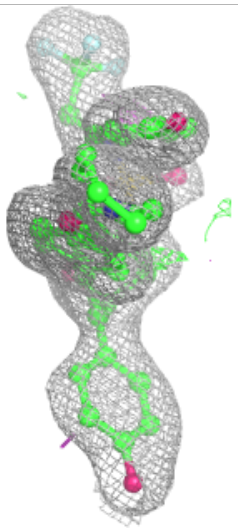


Electron density around 77I D 601:

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

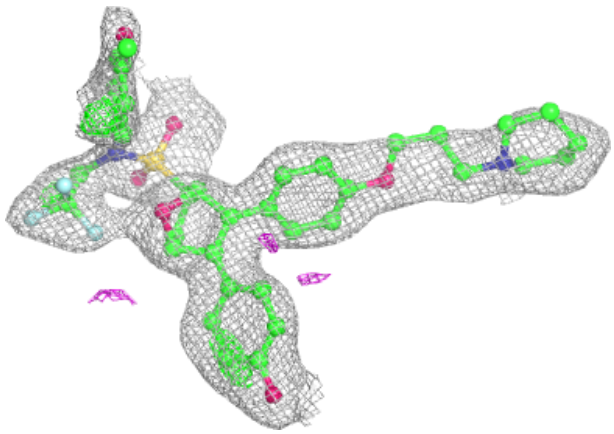


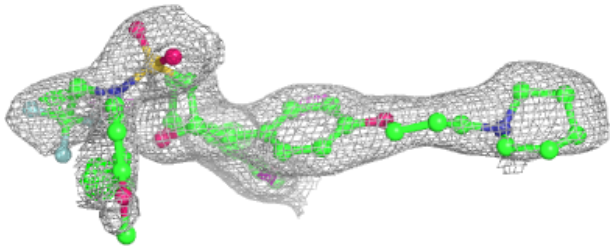


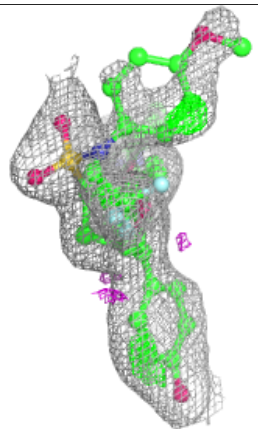


Electron density around 77I A 601 (A):

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

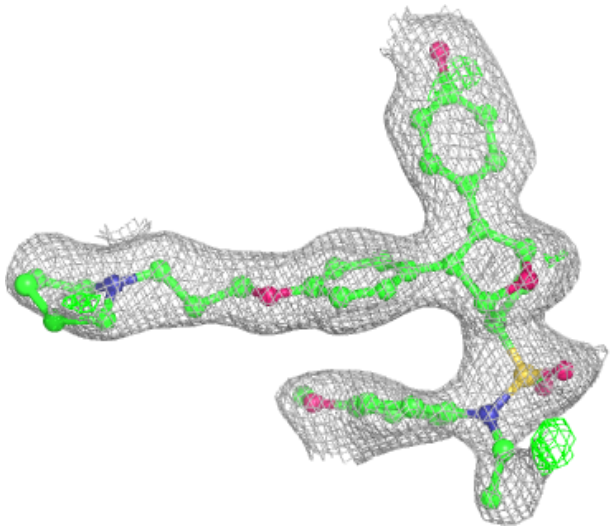


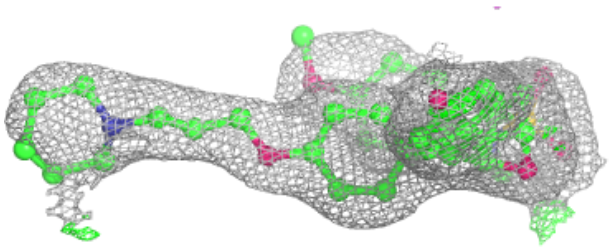


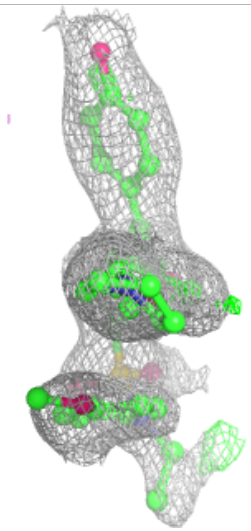


Electron density around 77I C 601:

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

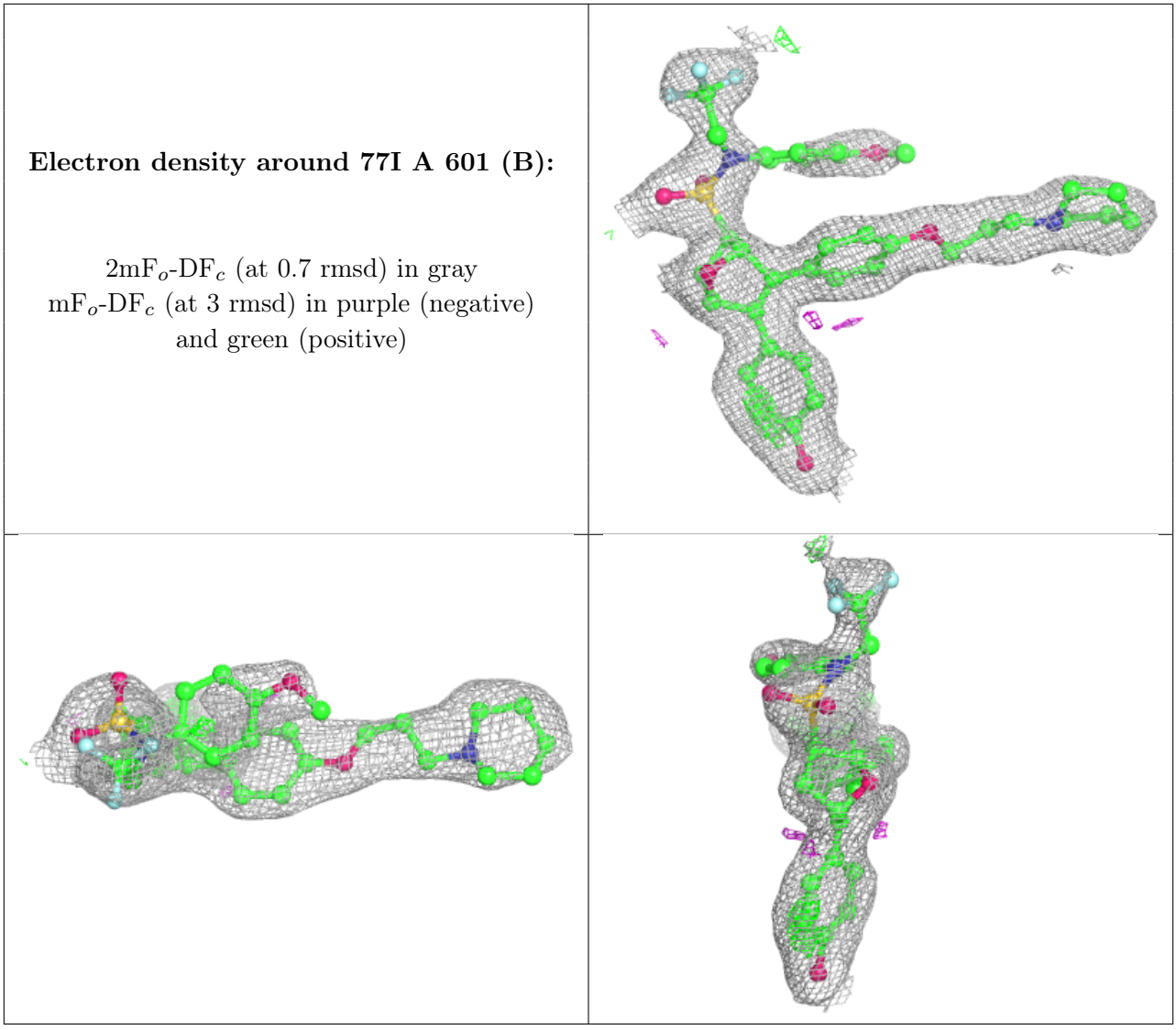






Electron density around 77I A 601 (B):

$2mF_o$-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.