



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 10:59 AM EDT

PDB ID : 7RRX
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with DMERI-19
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
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) : 2.23.1

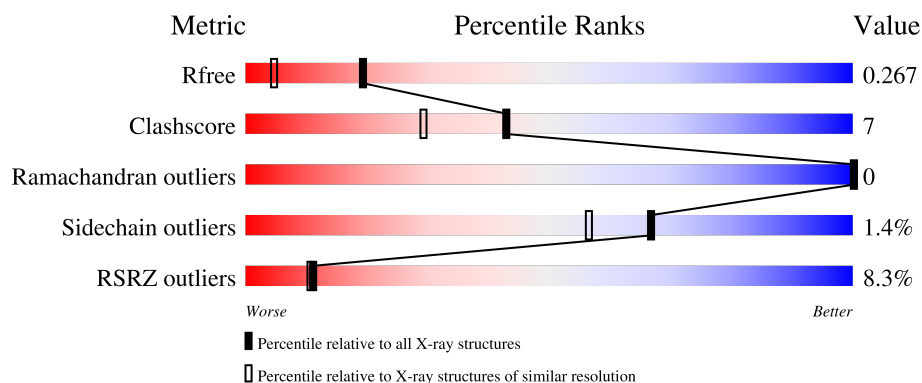
1 Overall quality at a glance

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 $\leq 5\%$. 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	257	
1	B	257	
1	C	257	
1	D	257	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7846 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.

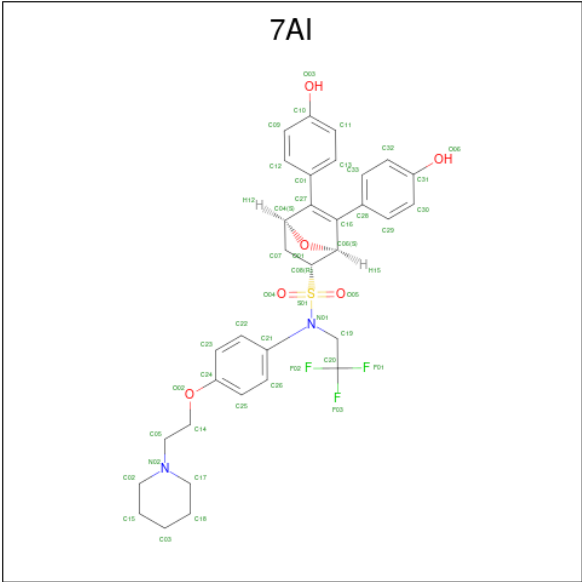
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1873	1199	316	341	17			
1	B	220	Total	C	N	O	S	0	0	0
			1767	1137	297	318	15			
1	C	234	Total	C	N	O	S	0	1	0
			1877	1198	319	341	19			
1	D	216	Total	C	N	O	S	0	0	0
			1726	1108	293	309	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)-5,6-bis(4-hydroxyphenyl)-N-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonamide (three-letter code: 7AI) (formula: C₃₃H₃₅F₃N₂O₆S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			45	33	3	2	6	1		
2	B	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		
2	C	1	Total	C	F	N	O	S	0	0
			45	33	3	2	6	1		
2	D	1	Total	C	F	N	O	S	0	0
			37	26	3	1	6	1		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	106	Total	O	0	0
			106	106		
4	C	103	Total	O	0	0
			103	103		

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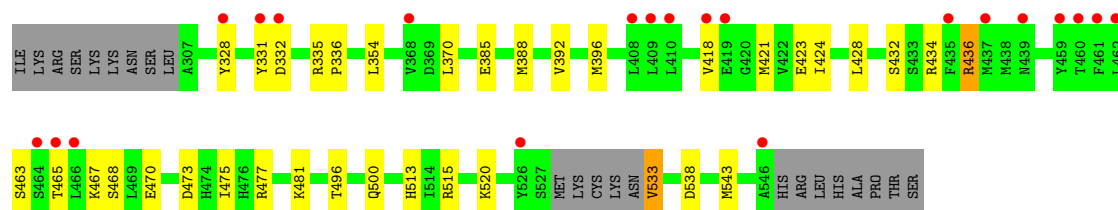
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	109	Total 109	O 109	0	0

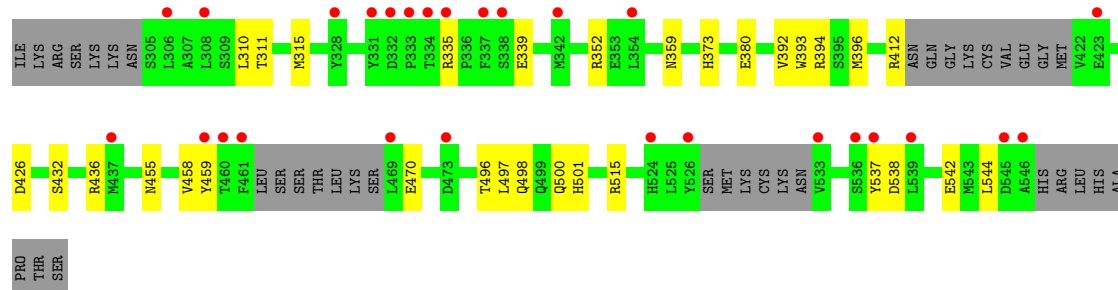
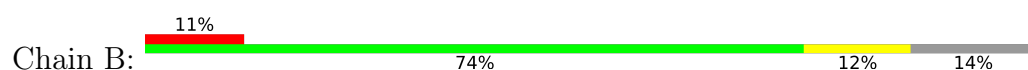
3 Residue-property plots [i](#)

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.

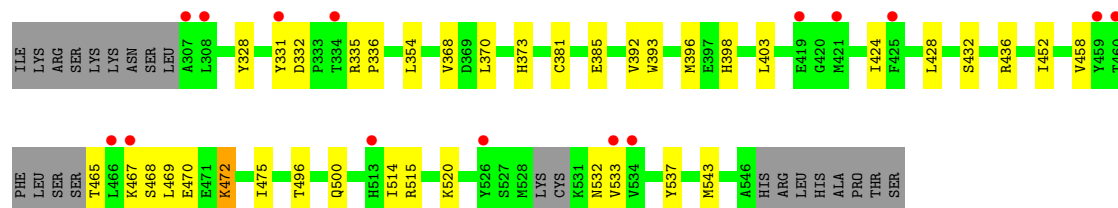
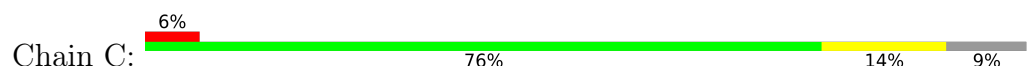
• Molecule 1: Estrogen receptor



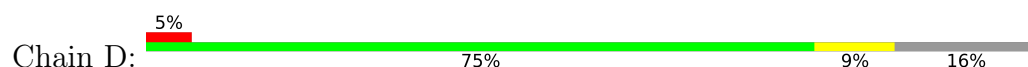
• Molecule 1: Estrogen receptor

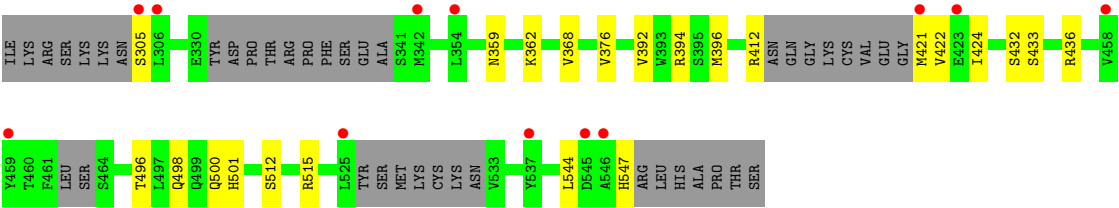


• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.78Å 58.75Å 94.44Å 86.91° 74.81° 62.77°	Depositor
Resolution (Å)	52.14 – 1.78 52.08 – 1.78	Depositor EDS
% Data completeness (in resolution range)	87.0 (52.14-1.78) 81.2 (52.08-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.236 , 0.265 0.243 , 0.267	Depositor DCC
R_{free} test set	3961 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.197 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7846	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 7.40% 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

5.1 Standard geometry

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

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	0.58	0/1897	0.74	4/2564 (0.2%)
1	B	0.58	0/1789	0.82	5/2418 (0.2%)
1	C	0.57	0/1889	0.73	0/2550
1	D	0.57	0/1743	0.76	4/2350 (0.2%)
All	All	0.57	0/7318	0.76	13/9882 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	394	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	515	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	D	515	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	D	515	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	515	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	394	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	515	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	515	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	352	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	538	ASP	CB-CG-OD1	-5.59	113.26	118.30
1	B	426	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	436	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	D	394	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1873	0	1909	38	2
1	B	1767	0	1799	25	2
1	C	1877	0	1913	31	1
1	D	1726	0	1774	12	1
2	A	45	0	0	8	0
2	B	37	0	0	0	0
2	C	45	0	0	4	0
2	D	37	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	119	0	0	2	0
4	B	106	0	0	6	0
4	C	103	0	0	1	0
4	D	109	0	0	2	0
All	All	7846	0	7395	100	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 (100) 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:B:310:LEU:HB3	4:B:701:HOH:O	1.58	1.01
1:C:385:GLU:HG3	1:C:514:ILE:HG22	1.41	1.00
1:A:428:LEU:HD12	2:A:601:7AI:F02	1.59	0.90
1:B:311:THR:O	4:B:701:HOH:O	1.89	0.89
1:C:428:LEU:HD12	2:C:601:7AI:F02	1.68	0.83
1:C:385:GLU:HG3	1:C:514:ILE:CG2	2.09	0.83
1:A:513:HIS:CD2	1:B:459:TYR:CD2	2.69	0.81
1:B:335:ARG:HB3	1:B:339:GLU:OE1	1.86	0.76
1:A:418:VAL:HG11	1:A:421:MET:CE	2.16	0.75
1:C:458:VAL:HG22	1:C:472:LYS:HE3	1.69	0.75
1:C:370:LEU:HD21	1:C:475:ILE:HD11	1.69	0.73
1:A:513:HIS:NE2	1:B:459:TYR:CD2	2.58	0.72
1:A:424:ILE:HD11	1:A:520:LYS:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HD21	1:A:475:ILE:HD11	1.74	0.68
1:C:465:THR:HG23	1:C:468:SER:H	1.58	0.67
1:C:424:ILE:HD11	1:C:520:LYS:HB3	1.76	0.67
1:A:428:LEU:CD1	2:A:601:7AI:F02	2.32	0.67
1:B:542:GLU:OE2	4:B:702:HOH:O	2.13	0.67
1:C:385:GLU:HG2	1:C:452:ILE:HD13	1.76	0.66
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.77	0.65
1:A:465:THR:HG23	1:A:468:SER:H	1.61	0.65
1:C:385:GLU:CG	1:C:514:ILE:HG22	2.21	0.64
1:A:513:HIS:NE2	1:B:459:TYR:HD2	1.95	0.64
1:A:473:ASP:OD1	1:A:477:ARG:NH1	2.31	0.63
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.80	0.63
1:C:396:MET:O	1:C:436:ARG:HD3	1.99	0.62
1:D:359:ASN:OD1	1:D:547:HIS:ND1	2.33	0.61
1:A:388:MET:HE2	2:A:601:7AI:S01	2.41	0.61
1:C:428:LEU:CD1	2:C:601:7AI:F02	2.39	0.61
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.83	0.61
1:A:396:MET:O	1:A:436:ARG:HD3	2.01	0.61
1:C:467:LYS:O	1:C:470:GLU:HG2	2.01	0.60
1:A:467:LYS:O	1:A:470:GLU:HG2	2.01	0.60
1:B:396:MET:O	1:B:436:ARG:HD3	2.02	0.59
1:A:533:VAL:HG23	2:A:601:7AI:O06	2.03	0.59
1:A:388:MET:HE2	2:A:601:7AI:O05	2.04	0.58
1:A:418:VAL:HG13	1:A:421:MET:CB	2.33	0.58
1:C:370:LEU:HD21	1:C:475:ILE:CD1	2.33	0.58
1:A:418:VAL:CG1	1:A:421:MET:SD	2.92	0.58
1:C:424:ILE:HD12	2:C:601:7AI:C23	2.36	0.56
1:A:513:HIS:CD2	1:B:459:TYR:CE2	2.94	0.56
1:B:380:GLU:OE1	4:B:703:HOH:O	2.18	0.55
1:A:385:GLU:OE1	4:A:701:HOH:O	2.18	0.55
1:A:428:LEU:HD11	2:A:601:7AI:O04	2.05	0.55
1:A:424:ILE:HD12	2:A:601:7AI:C23	2.38	0.53
1:C:373:HIS:HD2	1:C:537:TYR:OH	1.92	0.53
1:B:393:TRP:HE3	1:B:396:MET:HE1	1.74	0.53
1:D:368:VAL:HG22	4:D:751:HOH:O	2.08	0.53
1:B:393:TRP:CE3	1:B:396:MET:CE	2.93	0.51
1:B:315:MET:N	4:B:701:HOH:O	2.42	0.51
1:C:370:LEU:CD2	1:C:475:ILE:HD11	2.39	0.50
1:C:515:ARG:HD3	1:D:512:SER:O	2.12	0.50
1:B:393:TRP:CE3	1:B:396:MET:HE1	2.47	0.49
1:A:434:ARG:NH1	4:A:703:HOH:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:TYR:CE2	1:A:332:ASP:HB2	2.47	0.49
1:A:467:LYS:HA	1:A:470:GLU:OE2	2.12	0.48
1:A:418:VAL:HG13	1:A:421:MET:HB2	1.94	0.48
1:D:305:SER:N	4:D:704:HOH:O	2.46	0.48
1:C:331:TYR:CE2	1:C:332:ASP:HB2	2.48	0.48
1:B:373:HIS:NE2	1:B:537:TYR:OH	2.43	0.47
1:D:392:VAL:HG13	1:D:432:SER:HA	1.97	0.47
1:A:418:VAL:HG11	1:A:421:MET:SD	2.54	0.47
1:C:381[B]:YCM:HA	1:C:381[B]:YCM:NZ2	2.30	0.47
1:C:496:THR:O	1:C:500:GLN:HG3	2.15	0.46
1:B:310:LEU:CB	4:B:701:HOH:O	2.38	0.46
1:D:498:GLN:HA	1:D:501:HIS:CE1	2.51	0.46
1:C:424:ILE:HD11	1:C:520:LYS:CB	2.45	0.46
1:A:370:LEU:HD21	1:A:475:ILE:CD1	2.42	0.46
1:B:392:VAL:HG13	1:B:432:SER:HA	1.98	0.45
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.51	0.45
1:D:421:MET:SD	1:D:424:ILE:HG13	2.56	0.45
1:A:496:THR:O	1:A:500:GLN:HG3	2.16	0.45
1:A:513:HIS:HE1	1:B:455:ASN:O	1.99	0.45
1:B:496:THR:O	1:B:500:GLN:HG3	2.16	0.45
1:A:423:GLU:N	1:A:423:GLU:OE1	2.49	0.45
2:A:601:7AI:C07	2:A:601:7AI:C12	2.94	0.44
1:C:398:HIS:CE1	1:C:403:LEU:HD12	2.51	0.44
1:C:370:LEU:CD1	1:C:475:ILE:HD11	2.46	0.44
1:C:354:LEU:HD23	1:C:543:MET:HE1	1.99	0.44
2:C:601:7AI:C13	2:C:601:7AI:C07	2.95	0.44
1:A:513:HIS:CE1	1:B:459:TYR:HD2	2.37	0.43
1:A:513:HIS:NE2	1:B:459:TYR:CE2	2.86	0.43
1:D:496:THR:O	1:D:500:GLN:HG3	2.19	0.42
1:B:458:VAL:HG13	1:B:459:TYR:CD2	2.55	0.42
1:D:396:MET:O	1:D:436:ARG:NE	2.48	0.42
1:D:362:LYS:HG3	1:D:547:HIS:CD2	2.55	0.41
1:A:392:VAL:HG13	1:A:432:SER:HA	2.01	0.41
1:A:335:ARG:HA	1:A:336:PRO:C	2.39	0.41
1:C:335:ARG:HA	1:C:336:PRO:C	2.40	0.41
1:C:465:THR:CG2	1:C:468:SER:HB3	2.51	0.41
1:B:393:TRP:CE3	1:B:396:MET:HE3	2.56	0.41
1:C:393:TRP:CE3	1:C:396:MET:SD	3.14	0.41
1:C:458:VAL:CG2	1:C:472:LYS:HE3	2.46	0.41
1:A:354:LEU:HD23	1:A:543:MET:HE1	2.02	0.41
1:C:368:VAL:HG22	4:C:757:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:LYS:HE2	1:D:544:LEU:HD22	2.04	0.41
1:A:463:SER:HA	1:A:468:SER:OG	2.21	0.40
1:A:370:LEU:CD1	1:A:475:ILE:HD11	2.48	0.40
1:B:497:LEU:HD23	1:B:497:LEU:HA	1.92	0.40
1:C:392:VAL:HG13	1:C:432:SER:HA	2.02	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:A:481:LYS:NZ	1:B:538:ASP:OD2[1_655]	1.76	0.44
1:A:328:TYR:OH	1:B:359:ASN:ND2[1_565]	1.85	0.35
1:C:328:TYR:OH	1:D:359:ASN:ND2[1_645]	2.04	0.16

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	230/257 (90%)	226 (98%)	4 (2%)	0	100	100
1	B	211/257 (82%)	210 (100%)	1 (0%)	0	100	100
1	C	227/257 (88%)	225 (99%)	2 (1%)	0	100	100
1	D	205/257 (80%)	204 (100%)	1 (0%)	0	100	100
All	All	873/1028 (85%)	865 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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%)	209 (100%)	1 (0%)	88	86
1	B	197/231 (85%)	194 (98%)	3 (2%)	65	53
1	C	209/231 (90%)	205 (98%)	4 (2%)	57	43
1	D	194/231 (84%)	191 (98%)	3 (2%)	65	53
All	All	810/924 (88%)	799 (99%)	11 (1%)	67	56

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	533	VAL
1	B	412	ARG
1	B	470	GLU
1	B	544	LEU
1	C	469	LEU
1	C	472	LYS
1	C	532	ASN
1	C	533	VAL
1	D	412	ARG
1	D	422	VAL
1	D	433	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	455	ASN
1	A	519	ASN
1	B	398	HIS
1	B	476	HIS
1	B	519	ASN
1	C	373	HIS
1	C	398	HIS
1	C	498	GLN
1	C	519	ASN
1	D	373	HIS
1	D	439	ASN

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Mol	Chain	Res	Type
1	D	488	HIS
1	D	498	GLN
1	D	519	ASN
1	D	524	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	0.56	0	4,10,12	0.31	0
1	YCM	B	381	1	7,9,10	0.51	0	4,10,12	0.37	0
1	YCM	C	381[A]	1	7,9,10	0.48	0	4,10,12	0.51	0
1	YCM	A	381	1	7,9,10	0.57	0	4,10,12	0.47	0
1	YCM	C	381[B]	1	7,9,10	0.49	0	4,10,12	0.44	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	B	381	1	-	1/6/8/10	-
1	YCM	C	381[A]	1	-	1/6/8/10	-
1	YCM	A	381	1	-	1/6/8/10	-
1	YCM	C	381[B]	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) 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[A]	YCM	SG-CD-CE-NZ2
1	C	381[B]	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	C	381[B]	YCM	1	0

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	7AI	C	601	-	47,50,50	2.86	16 (34%)	61,74,74	2.80	21 (34%)
2	7AI	D	601	-	38,41,50	2.96	15 (39%)	50,63,74	3.04	15 (30%)
2	7AI	B	601	-	38,41,50	2.91	12 (31%)	50,63,74	2.93	14 (28%)
2	7AI	A	601	-	47,50,50	2.79	14 (29%)	61,74,74	2.52	22 (36%)

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	7AI	C	601	-	-	9/33/67/67	0/7/6/6
2	7AI	D	601	-	-	1/27/53/67	0/6/5/6
2	7AI	B	601	-	-	5/27/53/67	0/6/5/6
2	7AI	A	601	-	-	5/33/67/67	0/7/6/6

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	7AI	C21-N01	-11.07	1.29	1.44
2	C	601	7AI	C21-N01	-10.82	1.29	1.44
2	B	601	7AI	C21-N01	-10.71	1.29	1.44
2	D	601	7AI	C21-N01	-10.71	1.29	1.44
2	C	601	7AI	C06-C16	7.63	1.59	1.50
2	D	601	7AI	C28-C16	-6.51	1.36	1.48
2	B	601	7AI	C01-C27	-6.37	1.36	1.48
2	D	601	7AI	C01-C27	-6.29	1.36	1.48
2	A	601	7AI	C01-C27	-6.26	1.36	1.48
2	B	601	7AI	C28-C16	-5.89	1.37	1.48
2	A	601	7AI	C28-C16	-5.79	1.37	1.48
2	A	601	7AI	C06-C16	5.75	1.56	1.50
2	C	601	7AI	C28-C16	-5.74	1.37	1.48
2	C	601	7AI	C01-C27	-5.70	1.37	1.48
2	A	601	7AI	O05-S01	5.08	1.47	1.43
2	C	601	7AI	O04-S01	4.79	1.47	1.43
2	D	601	7AI	O04-S01	4.63	1.47	1.43
2	A	601	7AI	O04-S01	4.11	1.47	1.43
2	B	601	7AI	O04-S01	4.07	1.47	1.43
2	C	601	7AI	O05-S01	3.93	1.46	1.43
2	C	601	7AI	C07-C08	-3.65	1.49	1.54
2	B	601	7AI	C06-C16	3.54	1.54	1.50
2	B	601	7AI	S01-N01	3.32	1.74	1.67
2	D	601	7AI	S01-N01	3.21	1.74	1.67
2	B	601	7AI	O05-S01	3.12	1.46	1.43
2	D	601	7AI	O05-S01	3.07	1.46	1.43
2	A	601	7AI	S01-N01	2.94	1.73	1.67
2	D	601	7AI	C06-C16	2.90	1.53	1.50
2	B	601	7AI	C11-C10	-2.77	1.33	1.38
2	D	601	7AI	C11-C10	-2.73	1.33	1.38
2	A	601	7AI	C09-C10	-2.70	1.33	1.38
2	C	601	7AI	S01-N01	2.70	1.73	1.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	7AI	O01-C06	-2.65	1.40	1.43
2	A	601	7AI	C12-C09	-2.55	1.34	1.38
2	A	601	7AI	C22-C21	-2.53	1.34	1.39
2	D	601	7AI	C11-C13	-2.49	1.34	1.38
2	A	601	7AI	C23-C22	-2.43	1.34	1.38
2	B	601	7AI	C09-C10	-2.43	1.34	1.38
2	C	601	7AI	C11-C13	-2.42	1.34	1.38
2	A	601	7AI	C29-C28	-2.40	1.35	1.39
2	D	601	7AI	C30-C29	-2.37	1.34	1.38
2	D	601	7AI	C29-C28	-2.35	1.35	1.39
2	B	601	7AI	C23-C22	-2.33	1.34	1.38
2	D	601	7AI	O01-C06	-2.32	1.40	1.43
2	A	601	7AI	C30-C29	-2.26	1.34	1.38
2	C	601	7AI	C22-C21	-2.26	1.34	1.39
2	D	601	7AI	C12-C01	-2.21	1.35	1.39
2	C	601	7AI	C11-C10	-2.20	1.34	1.38
2	C	601	7AI	C29-C28	-2.20	1.35	1.39
2	D	601	7AI	C23-C22	-2.18	1.34	1.38
2	C	601	7AI	C30-C29	-2.18	1.34	1.38
2	A	601	7AI	C13-C01	-2.18	1.35	1.39
2	B	601	7AI	C11-C13	-2.18	1.34	1.38
2	C	601	7AI	C12-C01	-2.15	1.35	1.39
2	C	601	7AI	C27-C16	2.11	1.39	1.34
2	D	601	7AI	C30-C31	-2.05	1.35	1.38
2	B	601	7AI	C25-C26	-2.01	1.35	1.38

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	7AI	O04-S01-N01	-12.34	92.43	107.56
2	D	601	7AI	O05-S01-N01	-10.53	94.66	107.56
2	B	601	7AI	O05-S01-N01	-10.47	94.73	107.56
2	B	601	7AI	O04-S01-N01	-10.07	95.22	107.56
2	C	601	7AI	O04-S01-O05	-9.62	113.03	119.22
2	B	601	7AI	C20-C19-N01	9.50	121.37	112.14
2	D	601	7AI	C20-C19-N01	7.52	119.45	112.14
2	C	601	7AI	O04-S01-N01	-7.23	98.70	107.56
2	A	601	7AI	O04-S01-N01	-7.21	98.72	107.56
2	C	601	7AI	C04-C07-C08	-6.11	95.21	100.61
2	A	601	7AI	C26-C21-N01	6.04	129.17	120.16
2	A	601	7AI	O01-C04-C27	5.98	110.31	101.99
2	C	601	7AI	O05-S01-N01	-5.98	100.23	107.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	7AI	C28-C16-C06	5.65	130.56	121.27
2	C	601	7AI	C26-C21-N01	5.46	128.31	120.16
2	C	601	7AI	C20-C19-N01	5.36	117.35	112.14
2	D	601	7AI	C26-C21-N01	5.17	127.88	120.16
2	A	601	7AI	O05-S01-N01	-4.94	101.50	107.56
2	B	601	7AI	C26-C21-N01	4.62	127.05	120.16
2	A	601	7AI	O04-S01-O05	-4.57	116.28	119.22
2	A	601	7AI	C20-C19-N01	4.54	116.55	112.14
2	C	601	7AI	C25-C24-C23	-4.21	113.69	120.18
2	A	601	7AI	C01-C27-C16	4.13	139.51	128.81
2	C	601	7AI	C04-C27-C16	-3.96	98.65	106.97
2	A	601	7AI	C25-C24-C23	-3.93	114.12	120.18
2	C	601	7AI	O01-C04-C07	3.84	112.19	104.64
2	C	601	7AI	C01-C27-C16	3.61	138.16	128.81
2	D	601	7AI	O04-S01-O05	3.30	121.34	119.22
2	A	601	7AI	C04-C27-C16	-3.30	100.05	106.97
2	C	601	7AI	C12-C01-C13	-3.29	113.90	118.59
2	A	601	7AI	C23-C22-C21	3.18	124.51	120.32
2	C	601	7AI	C28-C16-C06	3.14	126.44	121.27
2	C	601	7AI	C01-C27-C04	-3.08	116.41	121.44
2	C	601	7AI	C11-C13-C01	3.02	124.29	120.78
2	A	601	7AI	C12-C01-C13	-3.00	114.31	118.59
2	A	601	7AI	C09-C12-C01	2.90	124.16	120.78
2	C	601	7AI	C33-C28-C29	-2.88	114.49	118.59
2	C	601	7AI	C23-C22-C21	2.85	124.07	120.32
2	C	601	7AI	C26-C25-C24	2.84	123.21	119.73
2	B	601	7AI	C22-C23-C24	2.78	122.93	119.88
2	A	601	7AI	C19-N01-C21	-2.74	113.94	117.59
2	C	601	7AI	F01-C20-C19	2.73	116.60	112.13
2	A	601	7AI	C26-C21-C22	-2.72	113.62	119.16
2	B	601	7AI	C33-C28-C29	-2.72	114.71	118.59
2	D	601	7AI	C01-C27-C16	2.66	135.68	128.81
2	C	601	7AI	C26-C21-C22	-2.62	113.84	119.16
2	B	601	7AI	C25-C24-C23	-2.60	115.39	119.77
2	B	601	7AI	C12-C01-C13	-2.57	114.93	118.59
2	D	601	7AI	C12-C01-C13	-2.53	114.98	118.59
2	D	601	7AI	C33-C28-C16	2.52	124.17	120.91
2	A	601	7AI	C26-C25-C24	2.48	122.77	119.73
2	D	601	7AI	C25-C24-C23	-2.48	115.59	119.77
2	B	601	7AI	C01-C27-C16	2.45	135.15	128.81
2	C	601	7AI	C22-C23-C24	2.38	122.65	119.73
2	A	601	7AI	C33-C28-C29	-2.37	115.20	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	7AI	C32-C31-C30	-2.36	115.79	119.77
2	D	601	7AI	O02-C24-C25	2.26	126.46	120.02
2	D	601	7AI	C22-C23-C24	2.25	122.35	119.88
2	B	601	7AI	C33-C28-C16	2.24	123.80	120.91
2	D	601	7AI	C29-C30-C31	2.21	122.29	119.88
2	A	601	7AI	C22-C23-C24	2.18	122.40	119.73
2	B	601	7AI	C26-C21-C22	-2.17	114.75	119.16
2	D	601	7AI	C33-C28-C29	-2.14	115.54	118.59
2	C	601	7AI	C32-C33-C28	2.13	123.26	120.78
2	A	601	7AI	C13-C01-C27	2.13	123.66	120.91
2	D	601	7AI	C26-C21-C22	-2.12	114.84	119.16
2	A	601	7AI	C18-C17-N02	2.10	114.69	111.33
2	B	601	7AI	O02-C24-C25	2.07	125.94	120.02
2	D	601	7AI	C32-C31-C30	-2.04	116.33	119.77
2	B	601	7AI	C25-C26-C21	2.01	122.97	120.32
2	A	601	7AI	C29-C28-C16	2.01	123.51	120.91
2	A	601	7AI	C22-C21-N01	-2.00	117.18	120.16

There are no chirality outliers.

All (20) torsion outliers are listed below:

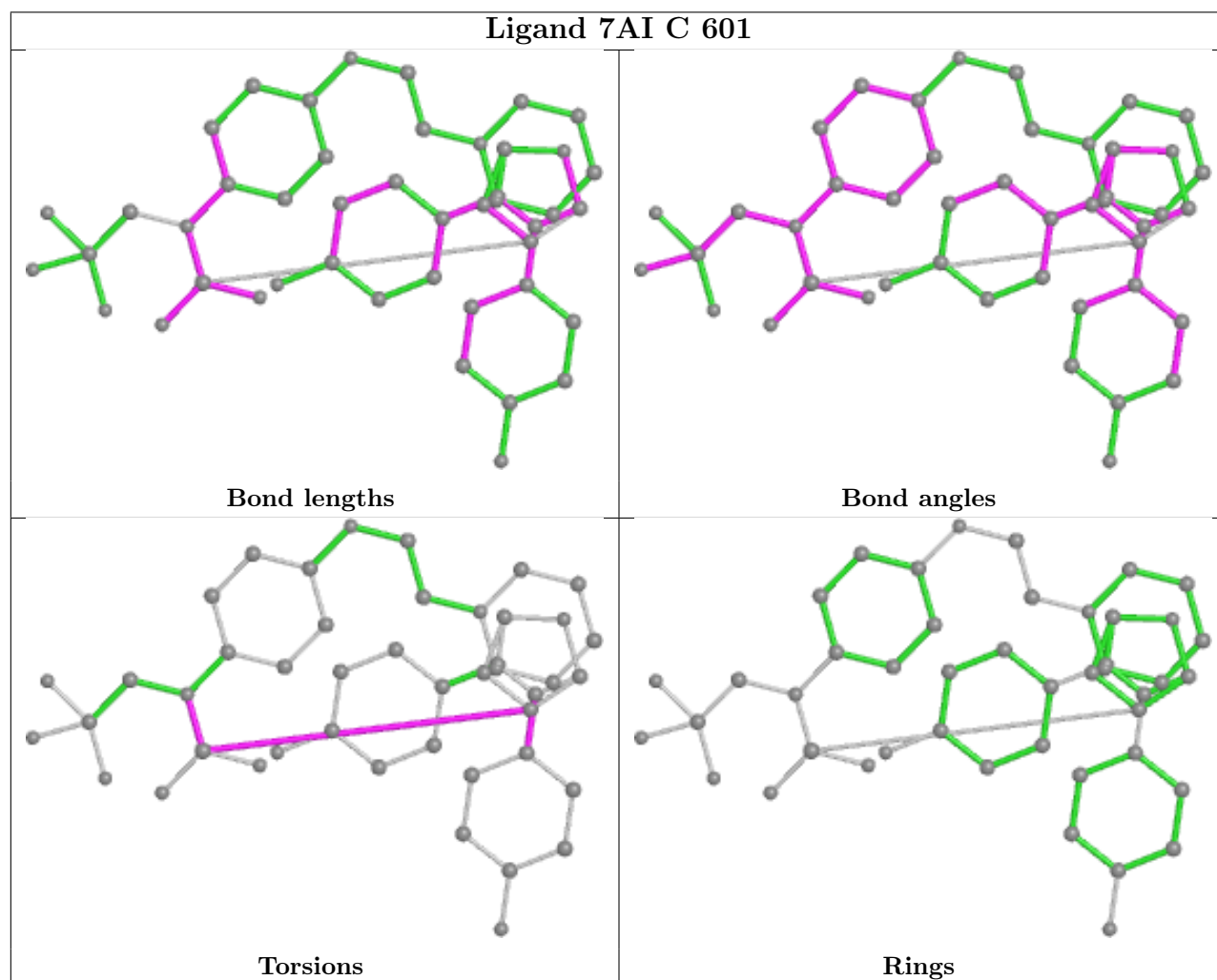
Mol	Chain	Res	Type	Atoms
2	A	601	7AI	C06-C08-S01-O04
2	B	601	7AI	C20-C19-N01-C21
2	B	601	7AI	C20-C19-N01-S01
2	B	601	7AI	C06-C08-S01-O05
2	C	601	7AI	C19-N01-S01-O05
2	C	601	7AI	C06-C08-S01-O05
2	C	601	7AI	C06-C08-S01-O04
2	C	601	7AI	C07-C08-S01-O04
2	D	601	7AI	C06-C08-S01-O05
2	C	601	7AI	C07-C08-S01-O05
2	A	601	7AI	C27-C16-C28-C29
2	B	601	7AI	C07-C08-S01-O05
2	C	601	7AI	C27-C16-C28-C29
2	C	601	7AI	C27-C16-C28-C33
2	B	601	7AI	C19-N01-S01-O04
2	A	601	7AI	C27-C16-C28-C33
2	A	601	7AI	C07-C08-S01-O04
2	A	601	7AI	C06-C08-S01-O05
2	C	601	7AI	C06-C16-C28-C29
2	C	601	7AI	C19-N01-S01-C08

There are no ring outliers.

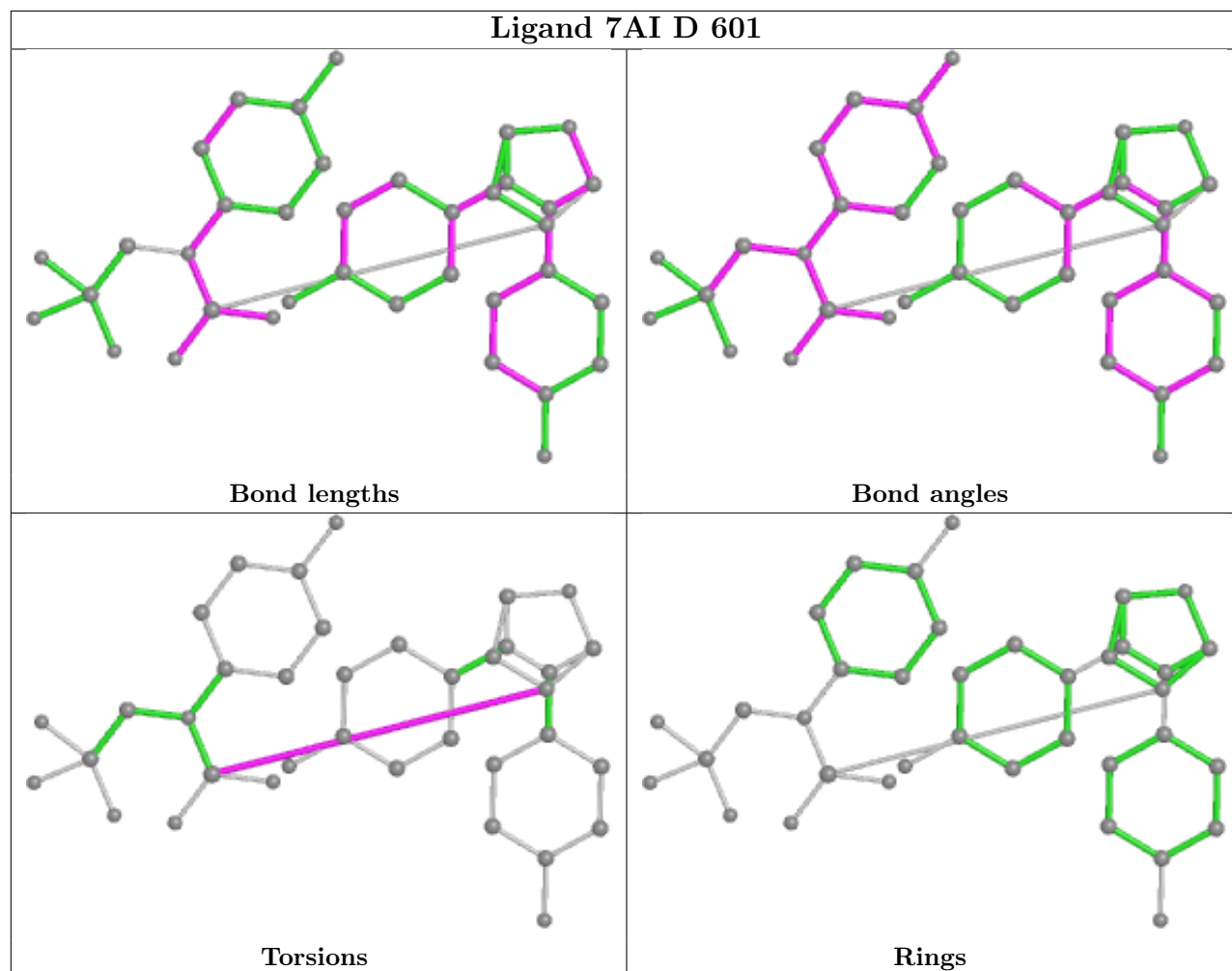
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	7AI	4	0
2	A	601	7AI	8	0

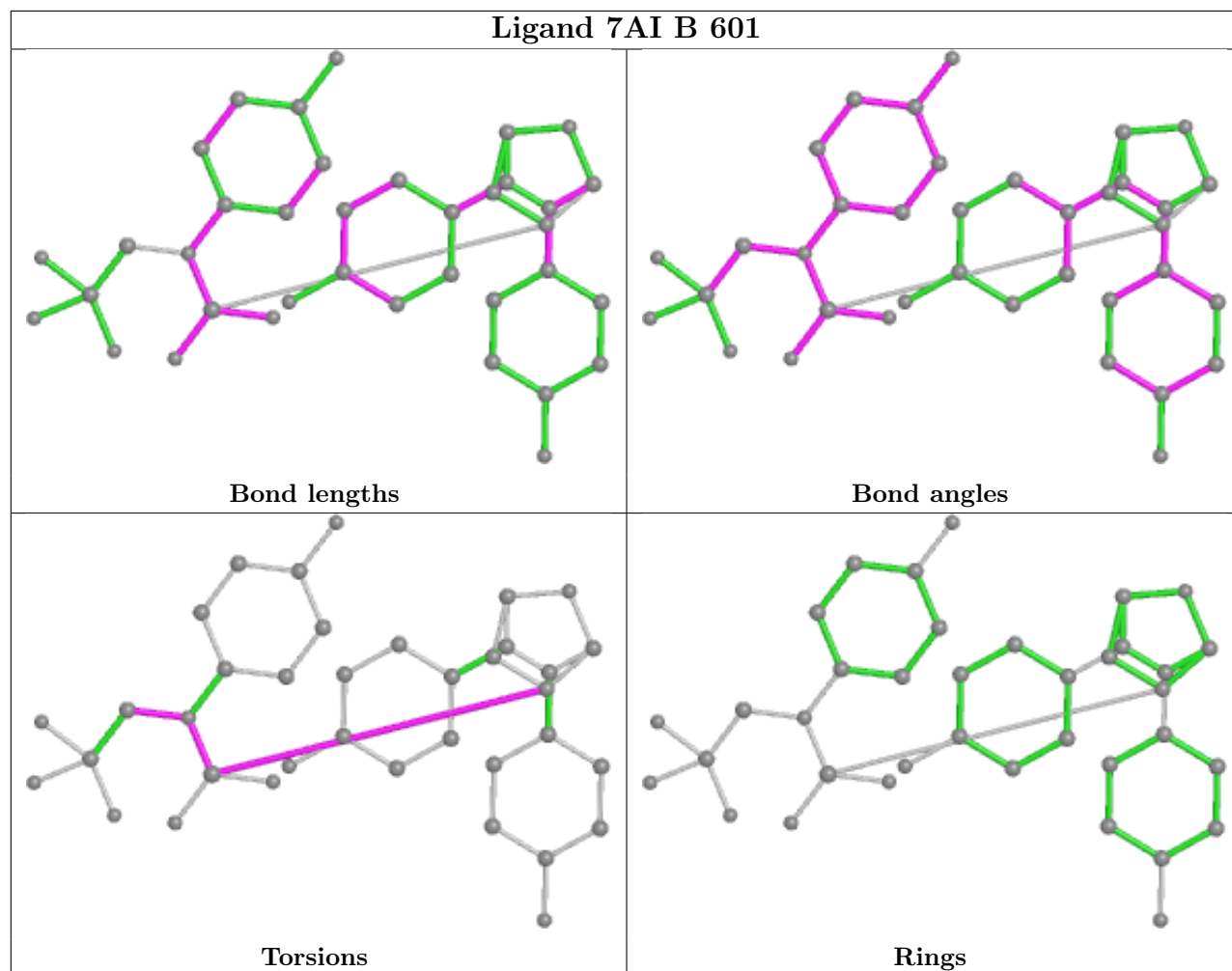
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

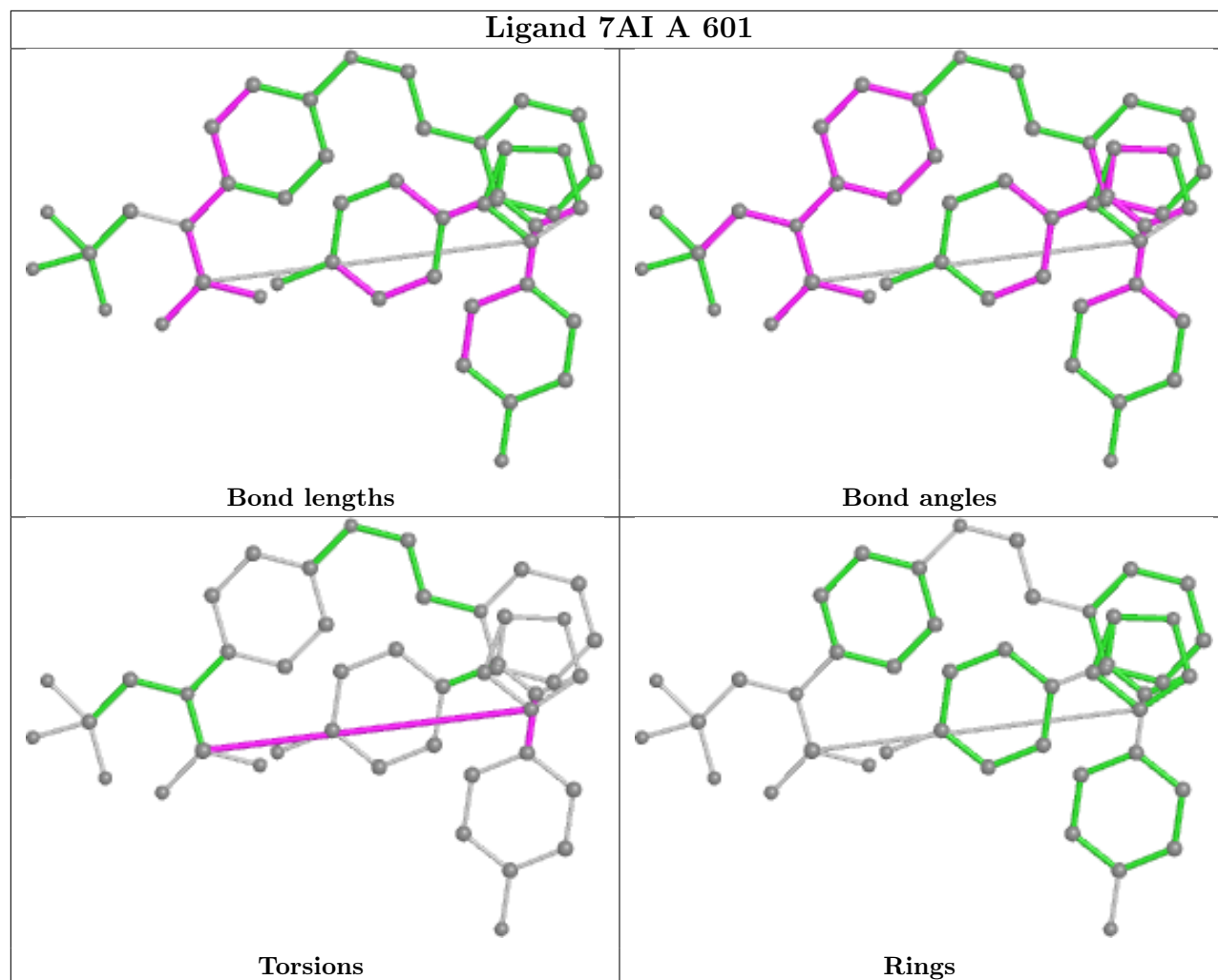


Ligand 7AI D 601



Ligand 7AI B 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 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	234/257 (91%)	0.78	21 (8%) 9 9	19, 33, 64, 83	0
1	B	219/257 (85%)	0.98	27 (12%) 4 4	19, 35, 56, 68	0
1	C	233/257 (90%)	0.72	15 (6%) 19 18	20, 35, 58, 82	0
1	D	215/257 (83%)	0.65	12 (5%) 24 23	20, 34, 53, 71	0
All	All	901/1028 (87%)	0.78	75 (8%) 11 11	19, 34, 57, 83	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	THR	6.3
1	C	466	LEU	6.2
1	B	337	PHE	6.0
1	A	462	LEU	6.0
1	B	333	PRO	6.0
1	B	331	TYR	5.8
1	B	461	PHE	5.6
1	B	459	TYR	5.3
1	A	526	TYR	5.2
1	B	524	HIS	4.8
1	A	460	THR	4.6
1	B	546	ALA	4.6
1	D	306	LEU	4.5
1	C	526	TYR	4.4
1	A	461	PHE	4.4
1	B	533	VAL	4.1
1	B	537	TYR	4.1
1	A	464	SER	3.9
1	D	342	MET	3.9
1	A	459	TYR	3.8
1	B	332	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	421	MET	3.8
1	C	331	TYR	3.5
1	A	331	TYR	3.5
1	A	418	VAL	3.4
1	B	536	SER	3.4
1	D	354	LEU	3.4
1	C	460	THR	3.2
1	C	425	PHE	3.2
1	B	342	MET	3.2
1	B	335	ARG	3.2
1	B	460	THR	3.2
1	A	332	ASP	3.1
1	C	307	ALA	3.1
1	A	408	LEU	3.1
1	B	545	ASP	3.1
1	B	338	SER	3.1
1	C	459	TYR	3.0
1	D	459	TYR	2.9
1	D	546	ALA	2.9
1	A	546	ALA	2.8
1	C	419	GLU	2.7
1	D	458	VAL	2.6
1	B	306	LEU	2.6
1	B	423	GLU	2.5
1	A	437	MET	2.5
1	C	334	THR	2.5
1	B	469	LEU	2.5
1	A	409	LEU	2.5
1	C	421	MET	2.4
1	D	545	ASP	2.4
1	A	435	PHE	2.4
1	B	437	MET	2.4
1	B	308	LEU	2.3
1	B	526	TYR	2.3
1	B	473	ASP	2.3
1	B	539	LEU	2.3
1	A	419	GLU	2.3
1	C	467	LYS	2.3
1	A	410	LEU	2.2
1	C	513	HIS	2.2
1	B	328	TYR	2.2
1	C	308	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	533	VAL	2.2
1	C	534	VAL	2.2
1	B	354	LEU	2.2
1	D	537	TYR	2.1
1	A	466	LEU	2.1
1	A	439	ASN	2.1
1	D	525	LEU	2.1
1	D	423	GLU	2.1
1	A	465	THR	2.1
1	A	328	TYR	2.1
1	D	305	SER	2.1
1	A	368	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	YCM	B	381	10/11	0.89	0.13	28,30,35,35	0
1	YCM	D	381	10/11	0.90	0.14	26,29,34,35	0
1	YCM	A	381	10/11	0.91	0.14	23,25,31,32	0
1	YCM	C	381[B]	10/11	0.94	0.13	23,25,29,31	10
1	YCM	C	381[A]	10/11	0.94	0.13	23,25,29,31	10

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	7AI	A	601	45/45	0.82	0.20	20,31,38,39	0

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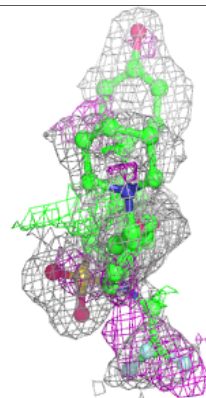
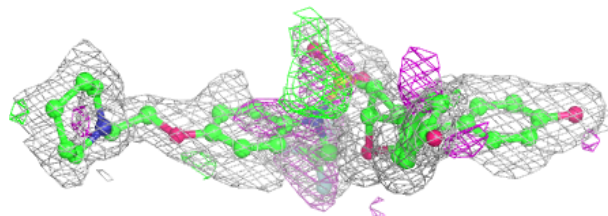
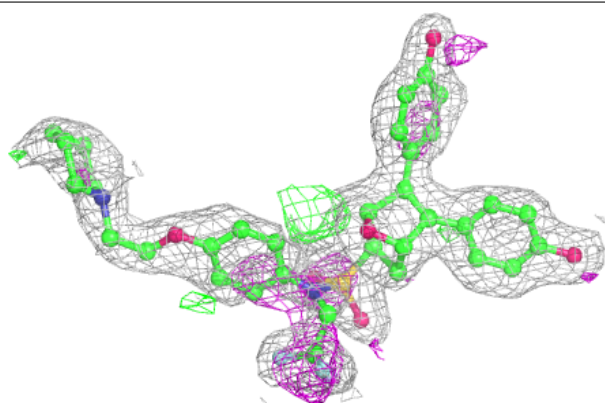
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	7AI	D	601	37/45	0.83	0.17	21,34,51,54	0
2	7AI	B	601	37/45	0.87	0.16	22,35,55,59	0
2	7AI	C	601	45/45	0.88	0.17	20,33,38,38	0
3	CL	B	602	1/1	0.96	0.05	26,26,26,26	0
3	CL	C	602	1/1	0.97	0.06	24,24,24,24	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.

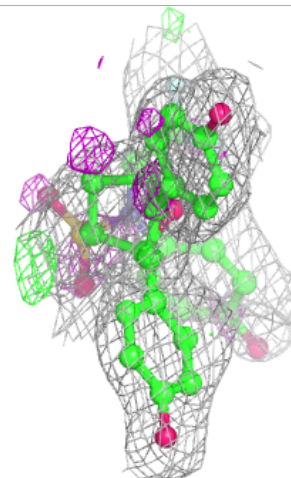
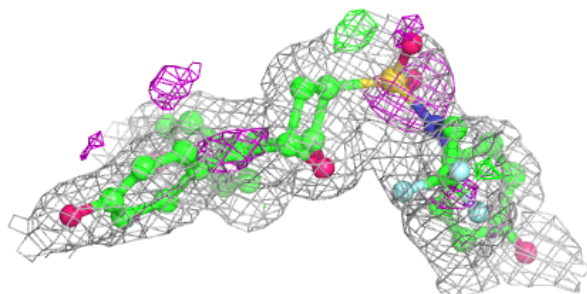
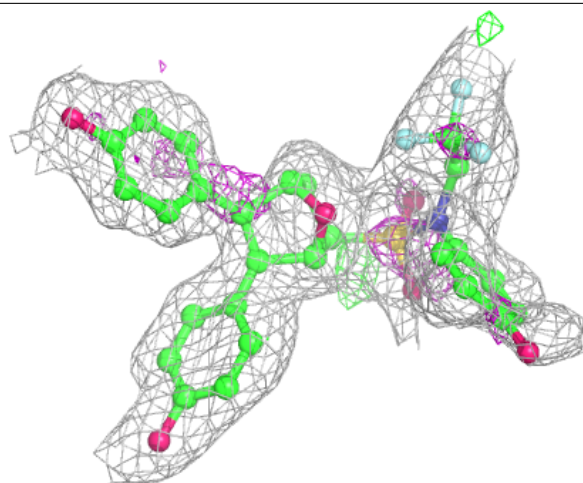
Electron density around 7AI A 601:

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



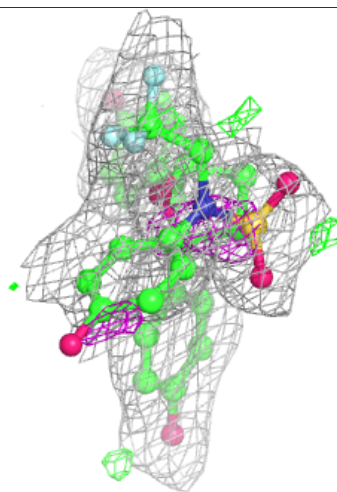
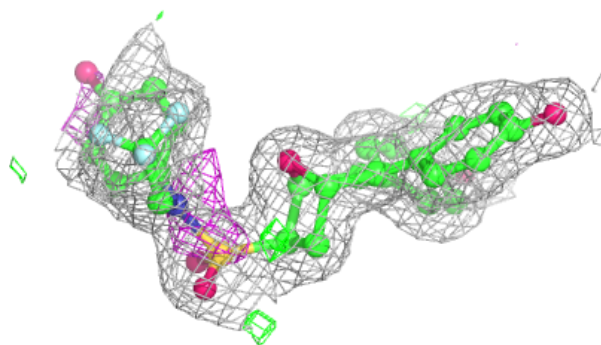
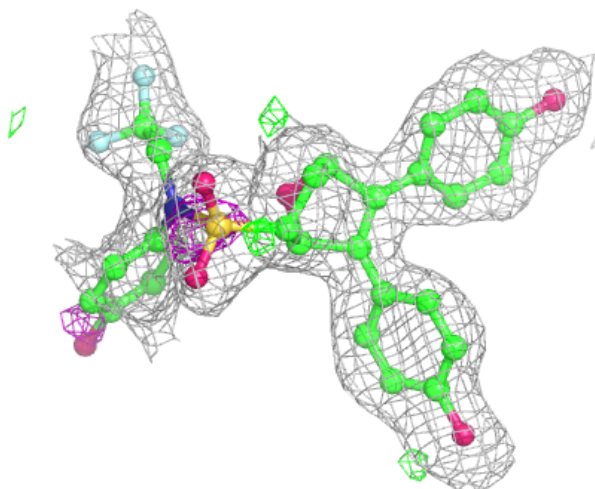
Electron density around 7AI D 601:

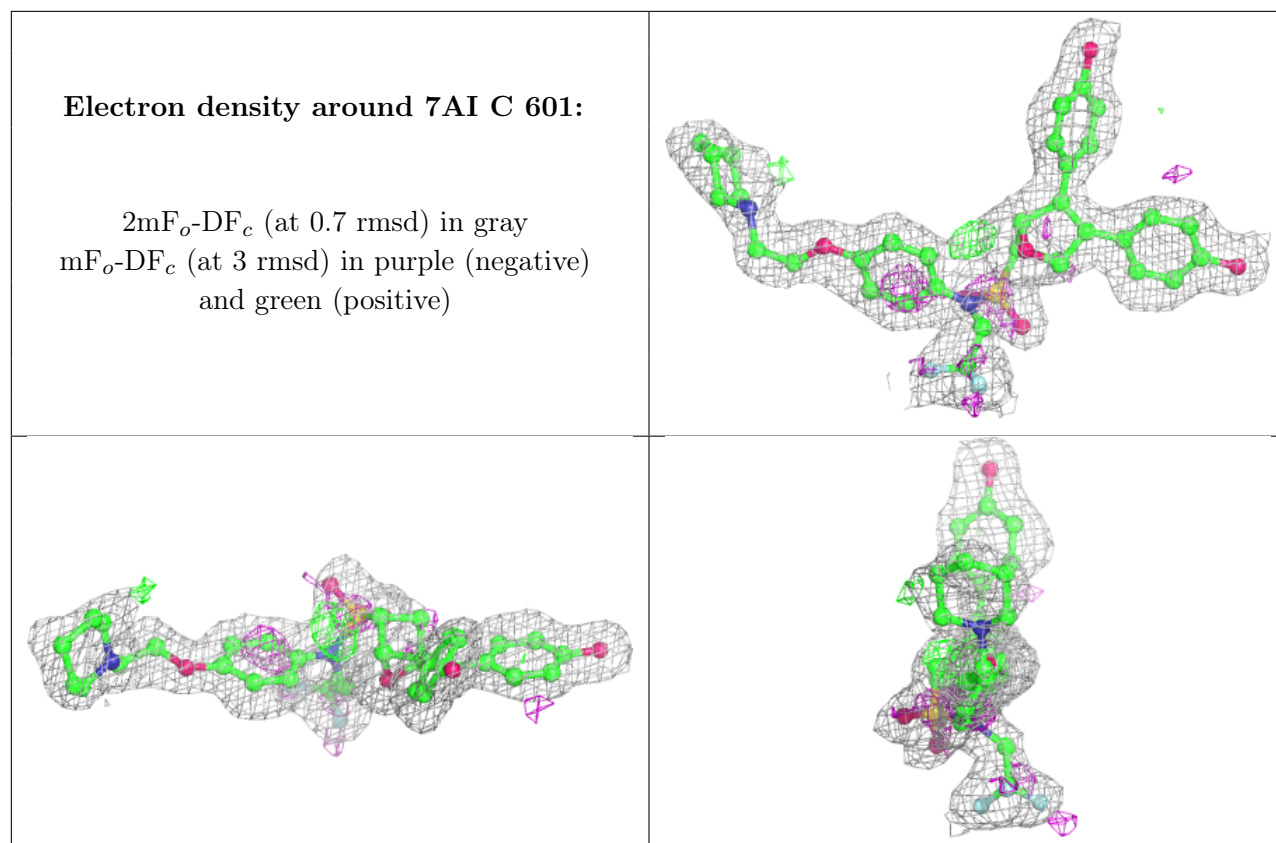
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7AI 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.