WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 4, 2024 – 08:14 PM EDT

PDB ID	:	8W03
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with k-1154
Authors	:	Min, C.K.; Nwachukwu, J.C.; Hou, Y.; Russo, R.J.; Papa, A.; Min, J.; Peng, R.; Kim, S.H.; Ziegler, Y.; Rangarajan, E.S.; Izard, T.; Katzenellenbogen, B.S.; Katzenellenbogen, J.A.; Nettles, K.W.
Deposited on	:	2024-02-13
Resolution	:	1.68 Å(reported)

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

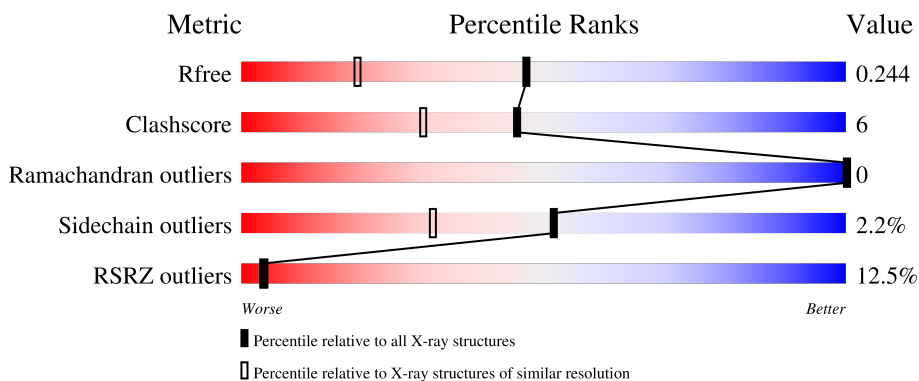|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.68 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	Percentile Ranks	Value
Rfree		0.244
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		2.2%
RSRZ outliers		12.5%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	242	11% / 83% / 15% ·
1	B	242	12% / 87% / 8% · ·
1	C	242	10% / 88% / 12%
1	D	242	15% / 81% / 11% / 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15422 atoms, of which 7505 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.
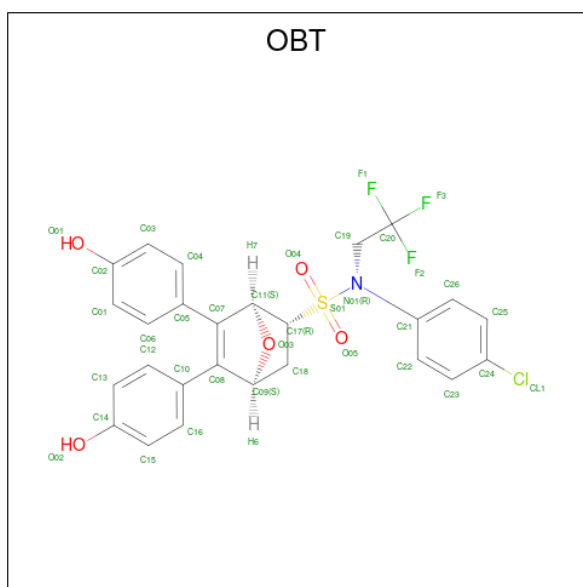
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	241	Total	C	H	N	O	S	0	1	0
			3758	1204	1876	322	339	17			
1	B	232	Total	C	H	N	O	S	0	0	0
			3663	1166	1843	309	330	15			
1	C	241	Total	C	H	N	O	S	0	1	0
			3804	1214	1906	322	345	17			
1	D	224	Total	C	H	N	O	S	0	0	0
			3579	1140	1802	303	318	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)-N-(4-chlorophenyl)-5,6-bis(4-hydroxyphenyl)-N-(2,2,2-trifluoroethyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonamide (three-letter code: OBT) (formula: $C_{26}H_{21}ClF_3NO_5S$) (labeled as "Ligand of Interest" by depositor).

OBT

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S		0	0
			40	18	15	1	5	1			
2	B	1	Total	C	Cl	H	N	O	S	0	0
			54	25	1	21	1	5	1		
2	C	1	Total	C	Cl	H	N	O	S	0	0
			54	25	1	21	1	5	1		
2	D	1	Total	C	Cl	F	H	N	O	S	0	0
			58	26	1	3	21	1	5	1		

- Molecule 3 is water.

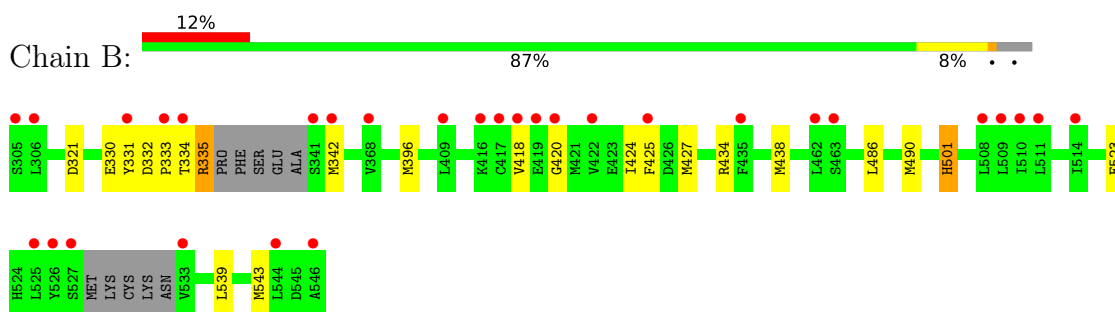| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		
3	B	109	Total	O	0	0
			109	109		
3	C	107	Total	O	0	0
			107	107		
3	D	90	Total	O	0	0
			90	90		

3 Residue-property plots ⓘ

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.
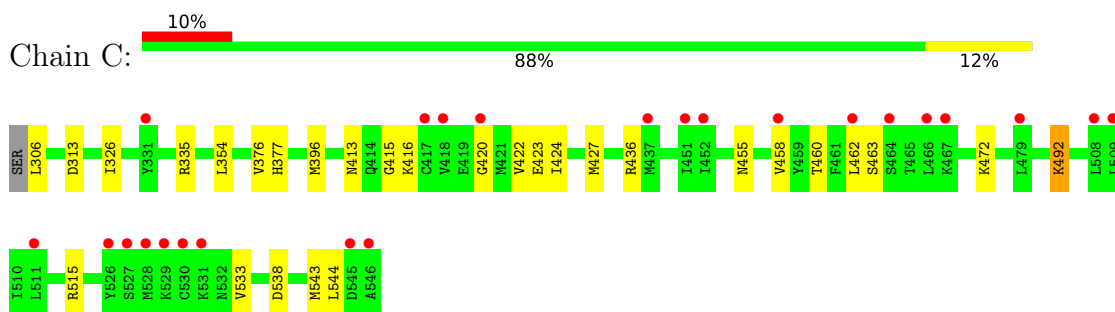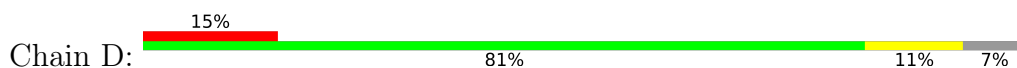
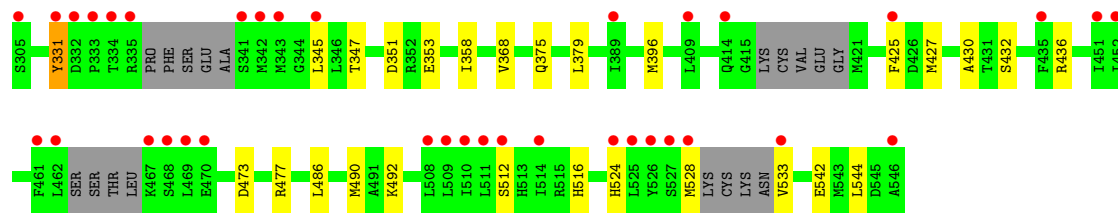- Molecule 1: Estrogen receptor
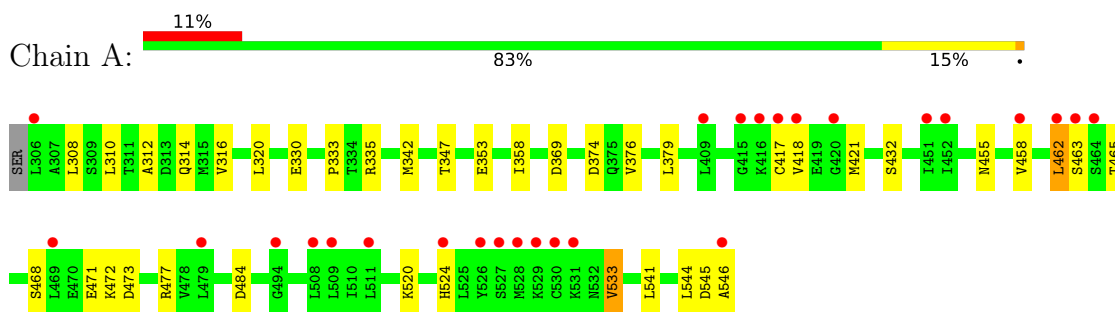
Chain A:

- Molecule 1: Estrogen receptor

Chain B:

- Molecule 1: Estrogen receptor

Chain C:

- Molecule 1: Estrogen receptor

Chain D:

S305 Y331 D332 P333 T334 R335 PRO PHE SER GLU ALA S341 M342 M343 G344 L345 L346 T347 D351 R352 E353 I358 V368 Q375 L379 I389 M396 L409 Q414 G415 LYS CYS VAL GLU GLY M421 F425 D426 M427 A430 T431 S432 F435 R436 I451 I452

F461 L462 SER SER THR LEU K467 S468 L469 E470 D473 R477 L486 M490 A491 K492 L508 L509 I510 L511 S512 H513 I514 R515 H516 H524 L525 Y526 S527 M528 LYS CYS LYS ASN V533 E542 M543 L544 D545 A546

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.49Å 58.77Å 93.21Å 86.61° 75.17° 62.96°	Depositor
Resolution (Å)	38.36 – 1.68 38.36 – 1.68	Depositor EDS
% Data completeness (in resolution range)	59.8 (38.36-1.68) 59.8 (38.36-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.04 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.201 , 0.245 0.202 , 0.244	Depositor DCC
R_{free} test set	3265 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 51.8	EDS
L-test for twinning[2]	$<|L|> = 0.51, <L^2> = 0.35$	Xtriage
Estimated twinning fraction	0.085 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15422	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 7.46% 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 (i)

5.1 Standard geometry (i)

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

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	0/1910	0.71	1/2589 (0.0%)
1	B	0.63	0/1840	0.69	0/2487
1	C	0.66	0/1926	0.71	0/2608
1	D	0.62	0/1796	0.69	0/2423
All	All	0.62	0/7472	0.70	1/10107 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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	462	LEU	CA-CB-CG	-5.45	102.77	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	LEU	Peptide

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	1882	1876	1875	34	0
1	B	1820	1843	1842	23	1
1	C	1898	1906	1904	20	0
1	D	1777	1802	1801	23	0
2	A	25	15	0	2	0
2	B	33	21	0	2	0
2	C	33	21	0	3	0
2	D	37	21	0	5	0
3	A	106	0	0	12	3
3	B	109	0	0	12	3
3	C	107	0	0	4	1
3	D	90	0	0	4	0
All	All	7917	7505	7422	95	4

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.

The worst 5 of 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:C:462:LEU:HD21	1:D:430:ALA:HB2	1.14	1.12
1:B:332:ASP:OD2	3:B:701:HOH:O	1.65	1.10
1:B:332:ASP:OD2	3:B:702:HOH:O	1.71	1.07
1:C:463:SER:OG	3:C:701:HOH:O	1.79	0.98
1:B:427:MET:SD	3:B:760:HOH:O	2.27	0.90

All (4) 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:B:333:PRO:O	3:C:701:HOH:O[1_466]	1.85	0.35
3:A:800:HOH:O	3:B:717:HOH:O[1_645]	1.95	0.25
3:A:785:HOH:O	3:B:808:HOH:O[1_645]	2.05	0.15
3:A:786:HOH:O	3:B:771:HOH:O[1_645]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/242 (99%)	236 (99%)	3 (1%)	0	100	100
1	B	225/242 (93%)	222 (99%)	3 (1%)	0	100	100
1	C	239/242 (99%)	236 (99%)	3 (1%)	0	100	100
1	D	213/242 (88%)	212 (100%)	1 (0%)	0	100	100
All	All	916/968 (95%)	906 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/217 (93%)	198 (98%)	4 (2%)	55	36
1	B	199/217 (92%)	194 (98%)	5 (2%)	47	26
1	C	207/217 (95%)	202 (98%)	5 (2%)	49	28
1	D	195/217 (90%)	191 (98%)	4 (2%)	53	33
All	All	803/868 (92%)	785 (98%)	18 (2%)	52	32

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	331	TYR
1	D	524	HIS
1	D	432	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	523	GLU
1	C	538	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	B	381	1	7,9,10	1.12	0	4,10,12	1.14	0
1	YCM	D	381	1	7,9,10	1.16	0	4,10,12	0.87	0
1	YCM	C	381	1	7,9,10	1.22	0	4,10,12	0.53	0
1	YCM	A	381	1	7,9,10	0.92	0	4,10,12	0.68	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	B	381	1	-	0/6/8/10	-
1	YCM	D	381	1	-	2/6/8/10	-
1	YCM	C	381	1	-	2/6/8/10	-
1	YCM	A	381	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	C	381	YCM	CE-CD-SG-CB
1	C	381	YCM	SG-CD-CE-NZ2
1	D	381	YCM	SG-CD-CE-NZ2
1	D	381	YCM	SG-CD-CE-OZ1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	OBT	D	600	-	38,41,41	3.16	13 (34%)	50,63,63	2.20	16 (32%)
2	OBT	C	600	-	34,37,41	3.12	17 (50%)	43,56,63	2.32	14 (32%)
2	OBT	B	600	-	34,37,41	2.59	15 (44%)	43,56,63	2.26	11 (25%)
2	OBT	A	600	-	26,28,41	2.61	10 (38%)	32,43,63	2.57	8 (25%)

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	OBT	D	600	-	-	9/27/53/53	0/6/5/5
2	OBT	C	600	-	-	9/22/48/53	0/6/5/5
2	OBT	B	600	-	-	8/22/48/53	0/6/5/5
2	OBT	A	600	-	-	4/12/38/53	0/5/4/5

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	OBT	C21-N01	-11.19	1.29	1.44
2	C	600	OBT	C19-N01	-9.40	1.29	1.47
2	D	600	OBT	C05-C07	-7.73	1.33	1.48
2	D	600	OBT	C10-C08	-7.35	1.34	1.48
2	A	600	OBT	C05-C07	-7.29	1.34	1.48

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	OBT	O05-S01-N01	10.52	119.75	107.08
2	C	600	OBT	O05-S01-N01	9.03	117.95	107.08
2	A	600	OBT	O04-S01-N01	8.89	116.94	107.72
2	A	600	OBT	O05-S01-N01	8.39	116.42	107.72
2	D	600	OBT	O04-S01-N01	7.74	117.03	107.56

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	OBT	C11-C17-S01-O04
2	B	600	OBT	C11-C17-S01-O05
2	B	600	OBT	C18-C17-S01-O04
2	B	600	OBT	C18-C17-S01-O05
2	B	600	OBT	C19-N01-S01-C17

There are no ring outliers.
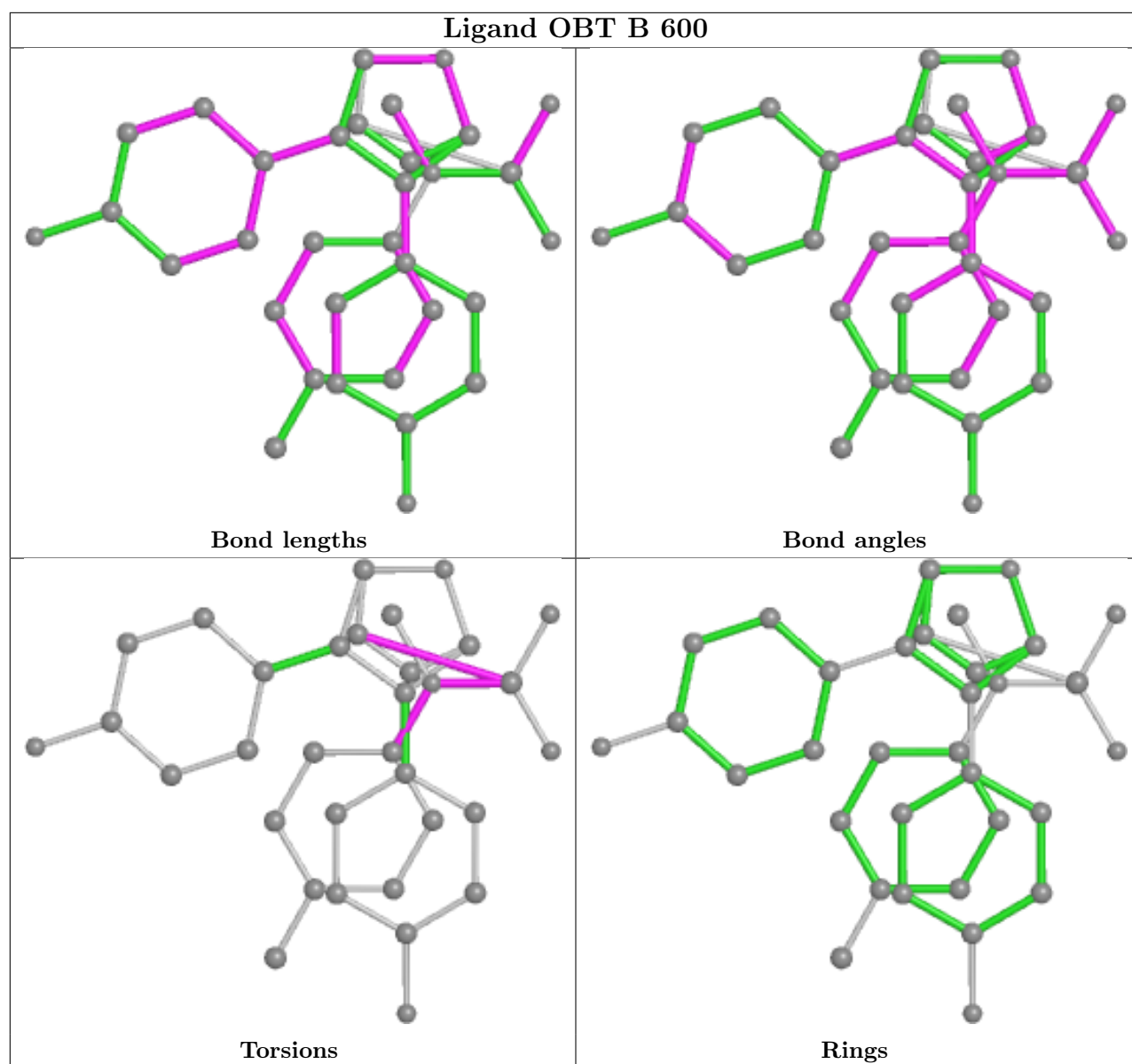
4 monomers are involved in 12 short contacts:

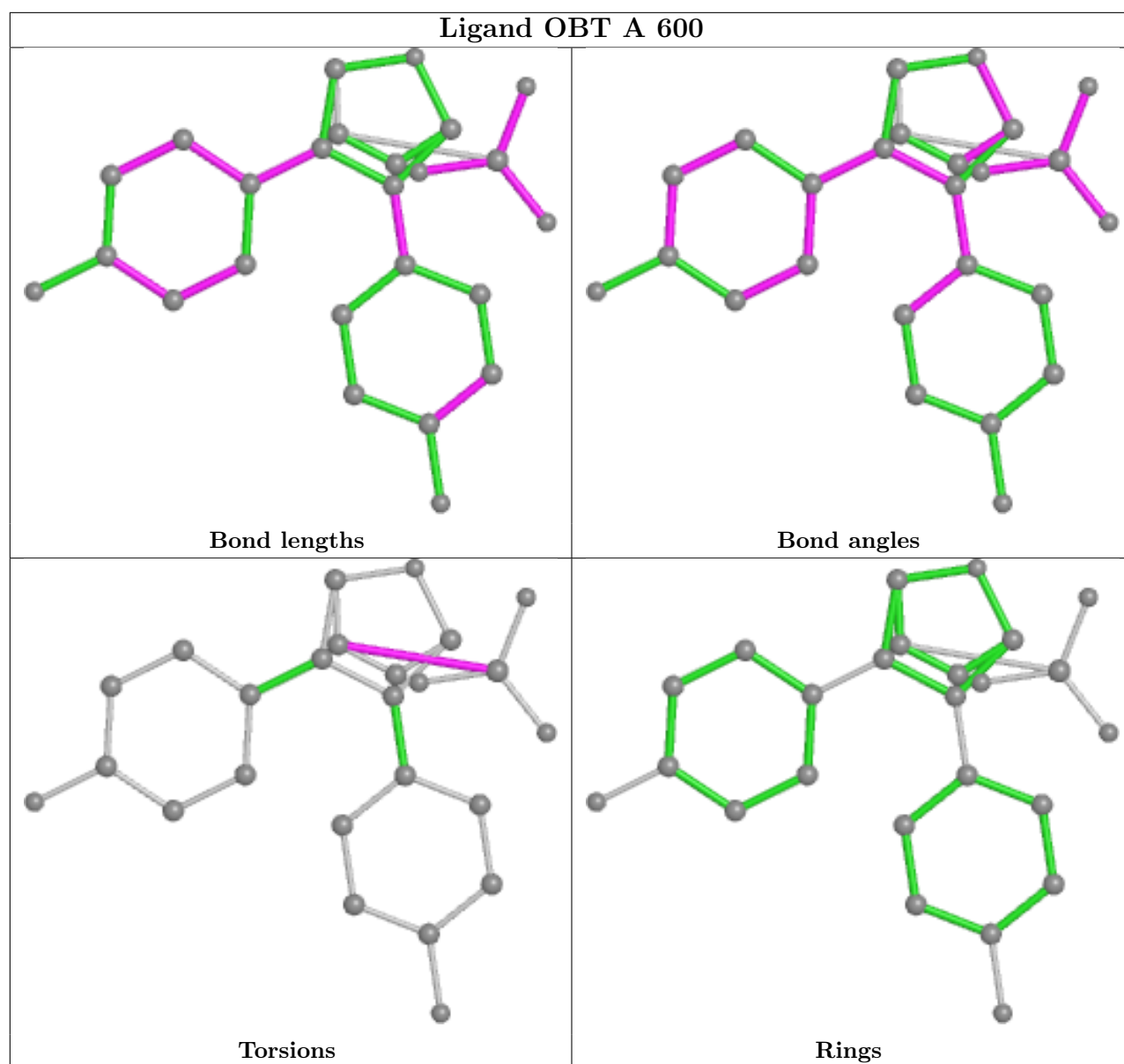| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	OBT	5	0
2	C	600	OBT	3	0
2	B	600	OBT	2	0
2	A	600	OBT	2	0

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 OBT D 600

Bond lengths

Bond angles

Torsions

Rings

Ligand OBT C 600

Bond lengths

Bond angles

Torsions

Rings

Ligand OBT B 600

Bond lengths

Bond angles

Torsions

Rings

Ligand OBT A 600

Bond lengths

Bond angles

Torsions

Rings
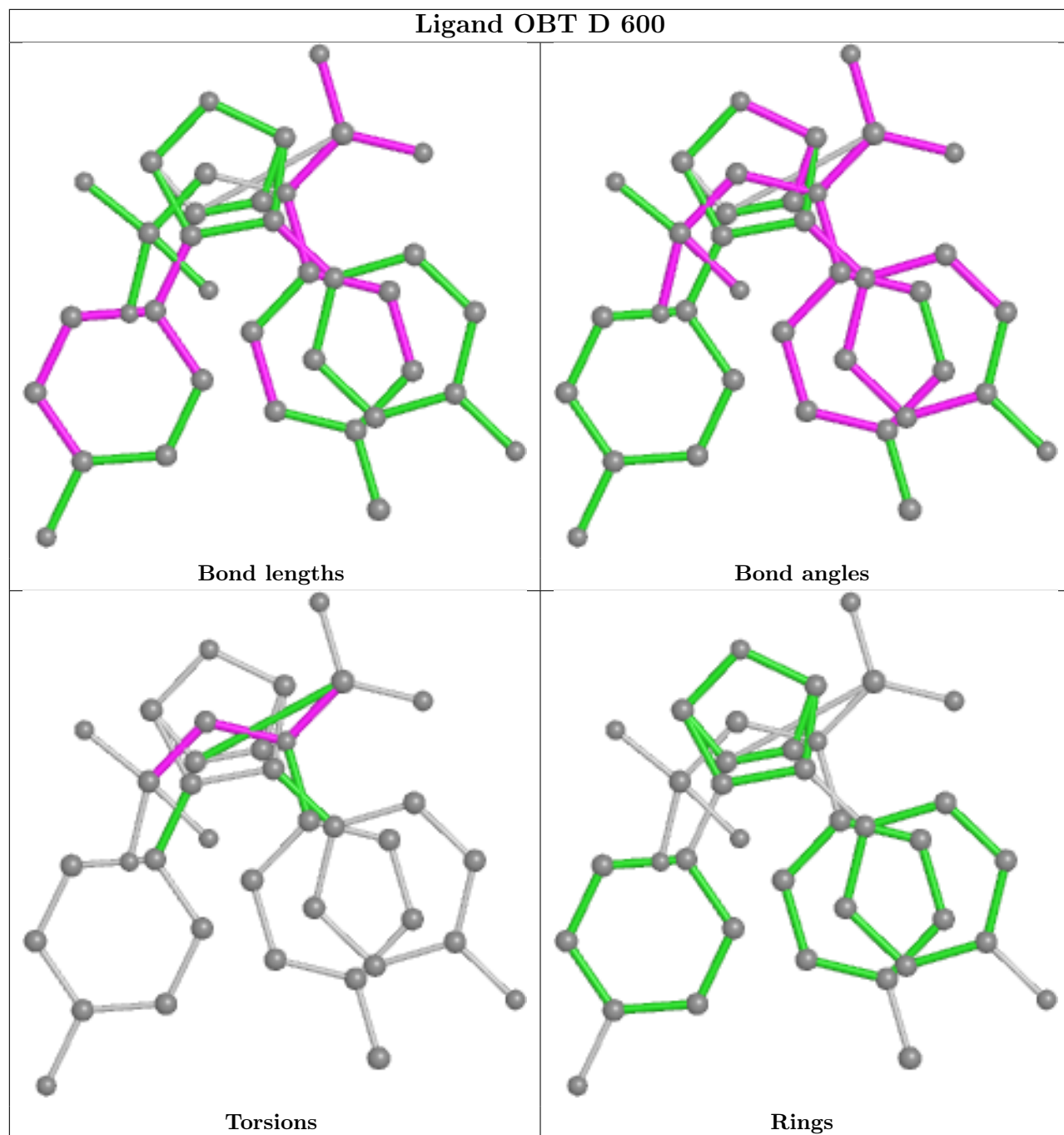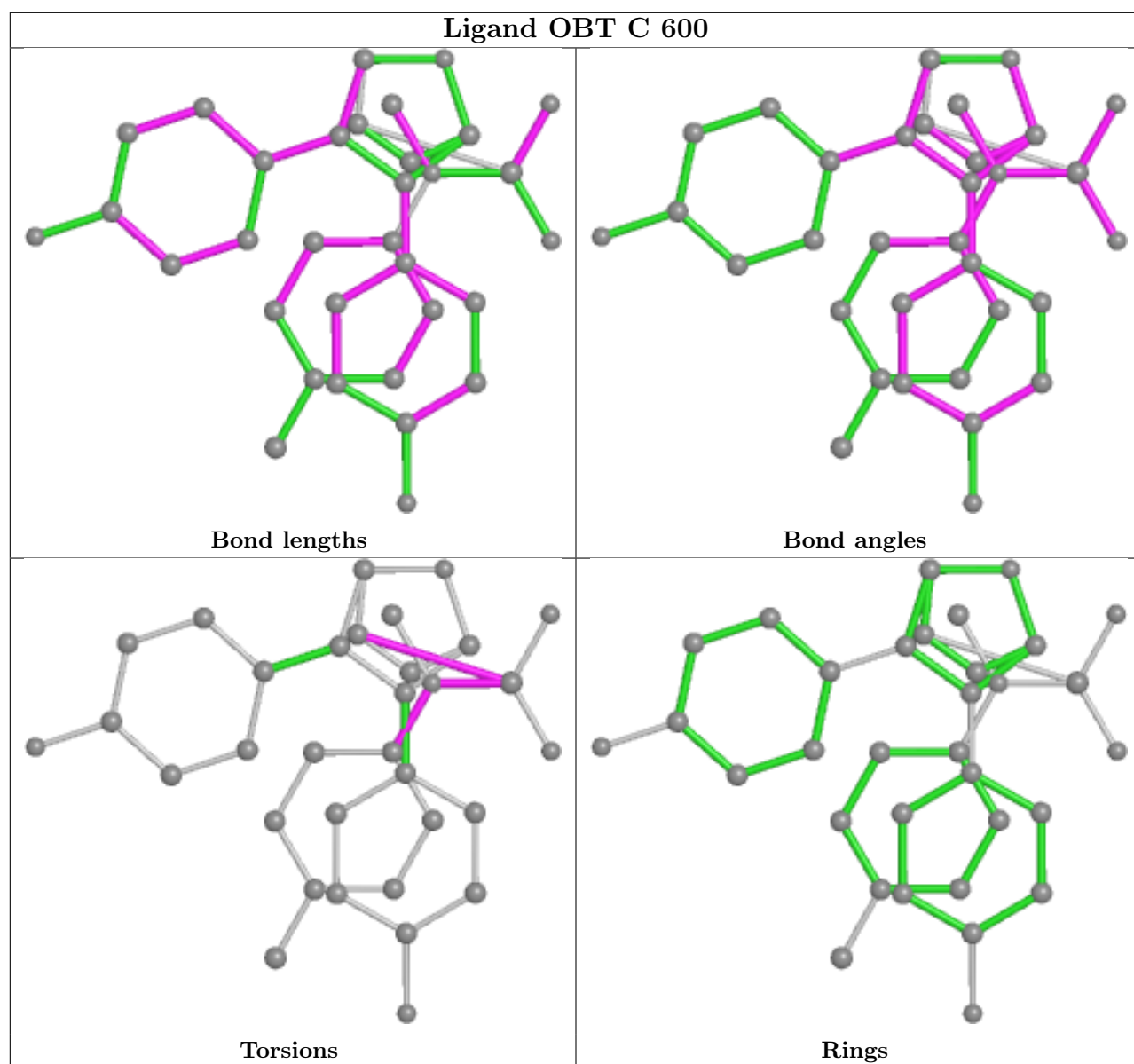
5.7 Other polymers ⓘ

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, 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	240/242 (99%)	0.74	27 (11%)	5	5	16, 32, 57, 95	0
1	B	231/242 (95%)	0.76	30 (12%)	3	3	15, 30, 73, 103	0
1	C	240/242 (99%)	0.63	24 (10%)	7	7	14, 29, 57, 76	0
1	D	223/242 (92%)	0.96	36 (16%)	1	1	15, 30, 69, 100	0
All	All	934/968 (96%)	0.77	117 (12%)	3	4	14, 30, 61, 103	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	462	LEU	14.8
1	D	331	TYR	8.3
1	B	526	TYR	8.2
1	B	417	CYS	7.9
1	A	526	TYR	7.4

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	C	381	10/11	0.92	0.16	19,26,54,54	0
1	YCM	D	381	10/11	0.94	0.14	24,36,60,60	0
1	YCM	A	381	10/11	0.95	0.13	14,25,45,45	0
1	YCM	B	381	10/11	0.96	0.11	18,29,43,43	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, 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	OBT	D	600	37/37	0.72	0.23	31,55,87,95	0
2	OBT	C	600	33/37	0.77	0.22	27,47,73,78	0
2	OBT	B	600	33/37	0.78	0.20	30,59,117,141	0
2	OBT	A	600	25/37	0.81	0.16	27,40,56,66	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.

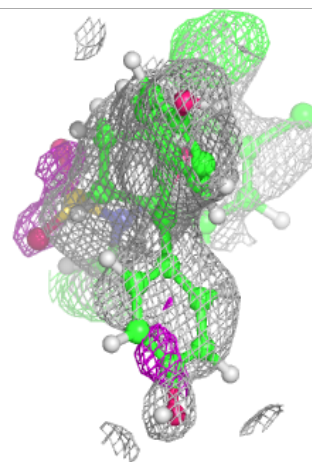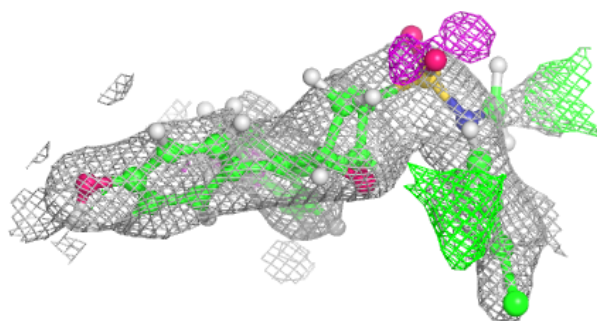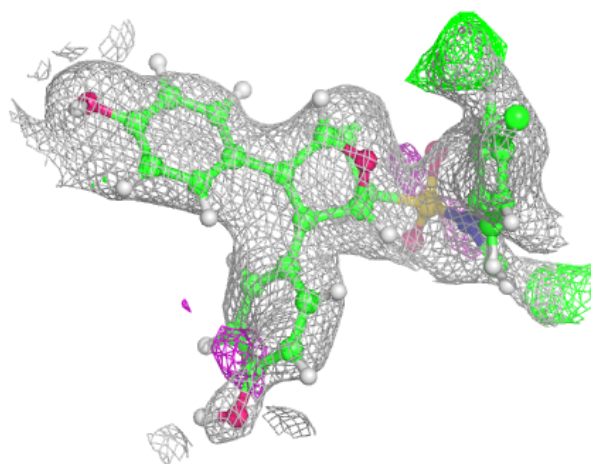**Electron density around OBT D 600:**

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

Electron density around OBT C 600:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
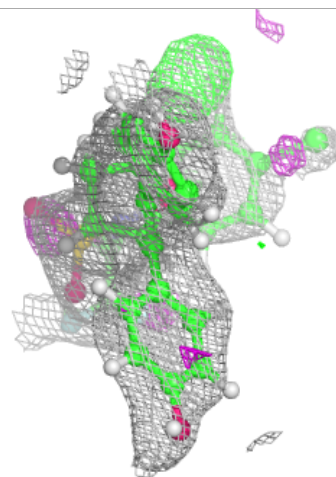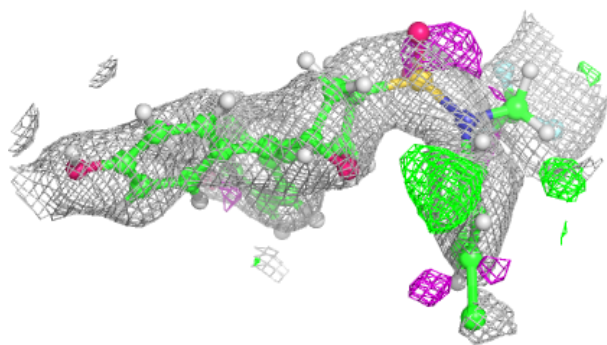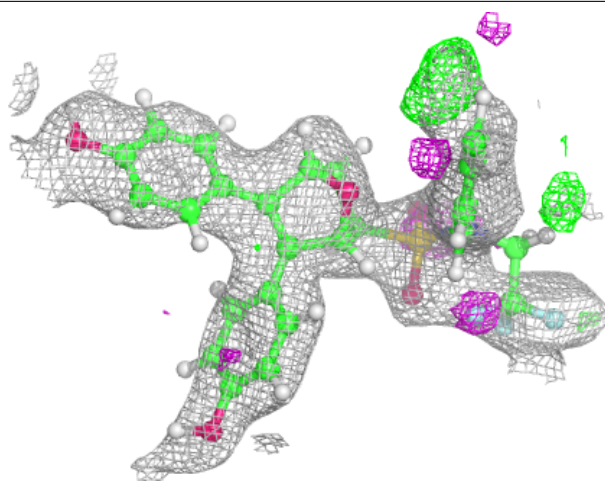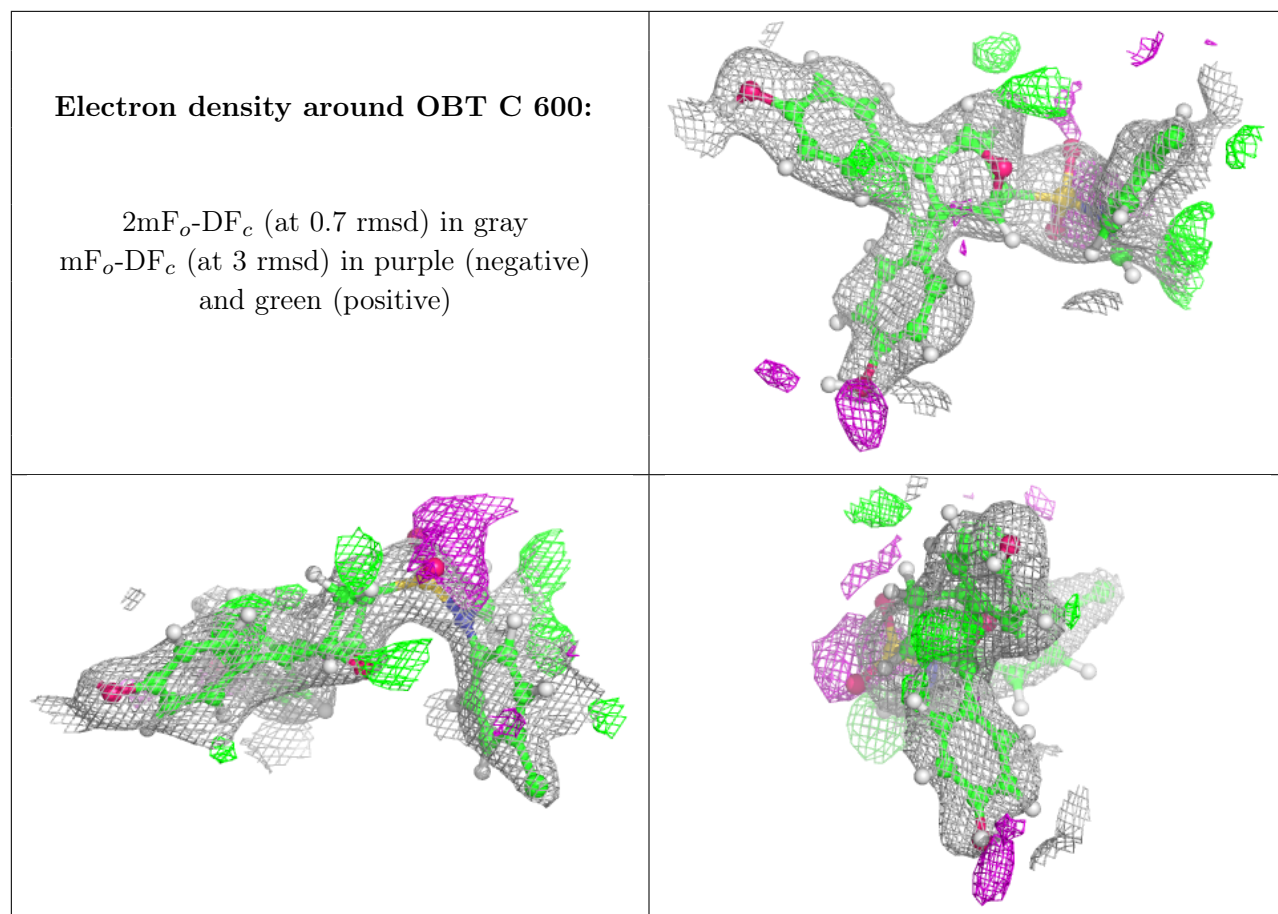
Electron density around OBT B 600:

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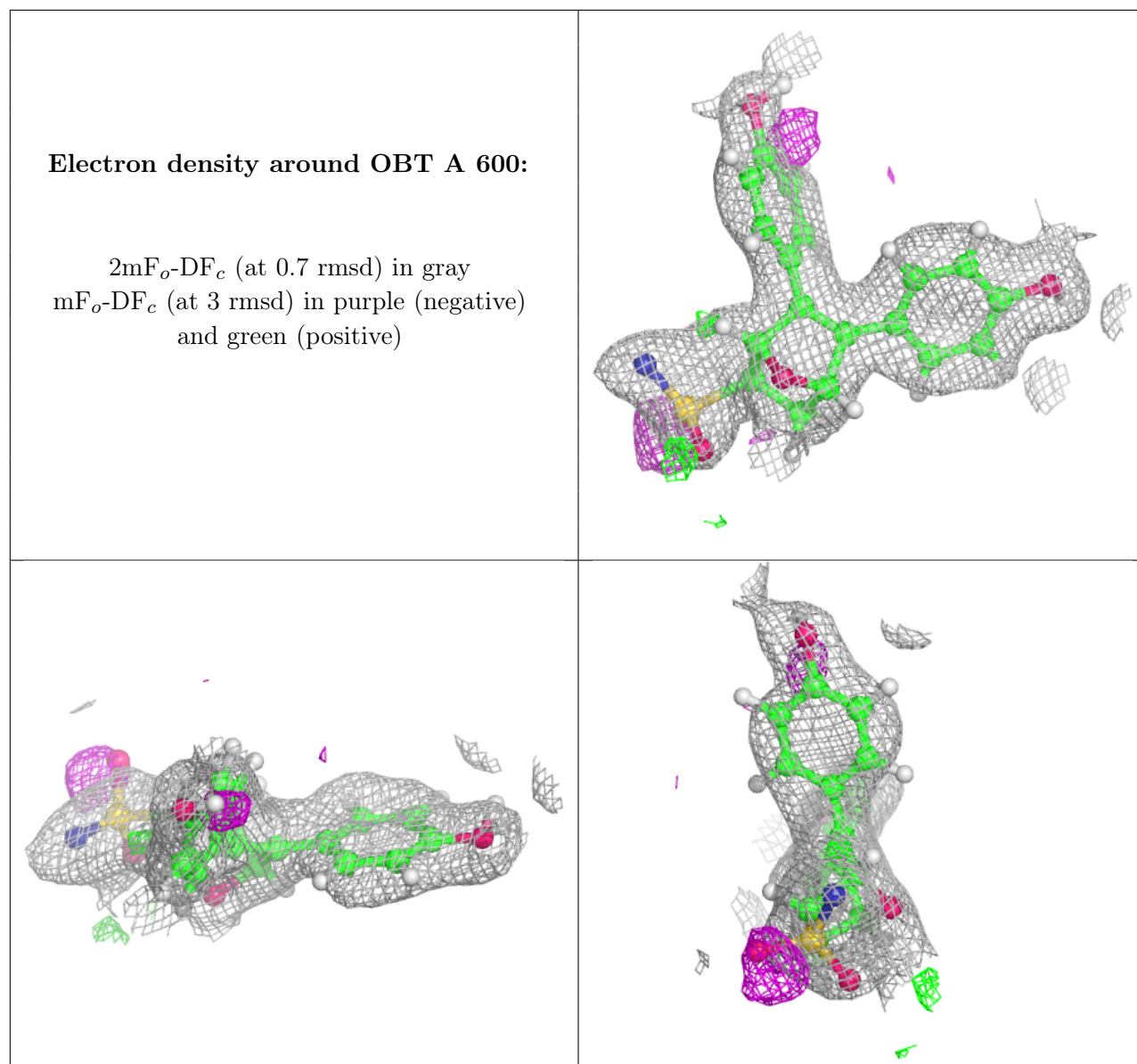$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around OBT A 600:

$2mF_o$-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.