



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 09:08 PM JST

PDB ID : 7XVY
Title : Human Estrogen Receptor beta Ligand-binding Domain in Complex with S-DPN
Authors : Furuya, N.; Handa, C.
Deposited on : 2022-05-25
Resolution : 1.54 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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

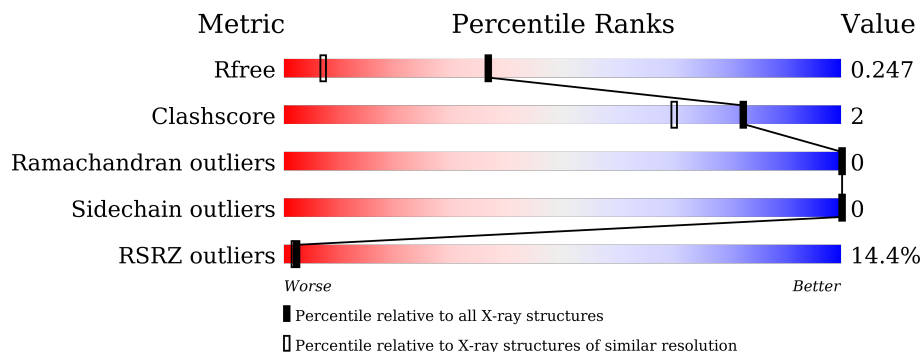
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	247	 13% 83% 5% 11%
1	B	247	 13% 86% . 9%
2	C	13	 15% 77% 8% 15%
2	D	13	 69% 8% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7668 atoms, of which 3728 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 beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	219	3479	1096	1769	286	310	18	95	4	1
1	B	224	3468	1101	1752	287	311	17	100	2	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	GLY	-	expression tag	UNP Q92731
A	257	PRO	-	expression tag	UNP Q92731
A	258	LEU	-	expression tag	UNP Q92731
A	259	GLY	-	expression tag	UNP Q92731
A	260	SER	-	expression tag	UNP Q92731
A	334	SER	CYS	engineered mutation	UNP Q92731
A	369	SER	CYS	engineered mutation	UNP Q92731
A	481	SER	CYS	engineered mutation	UNP Q92731
A	501	ASP	-	expression tag	UNP Q92731
A	502	ASP	-	expression tag	UNP Q92731
B	256	GLY	-	expression tag	UNP Q92731
B	257	PRO	-	expression tag	UNP Q92731
B	258	LEU	-	expression tag	UNP Q92731
B	259	GLY	-	expression tag	UNP Q92731
B	260	SER	-	expression tag	UNP Q92731
B	334	SER	CYS	engineered mutation	UNP Q92731
B	369	SER	CYS	engineered mutation	UNP Q92731
B	481	SER	CYS	engineered mutation	UNP Q92731
B	501	ASP	-	expression tag	UNP Q92731
B	502	ASP	-	expression tag	UNP Q92731

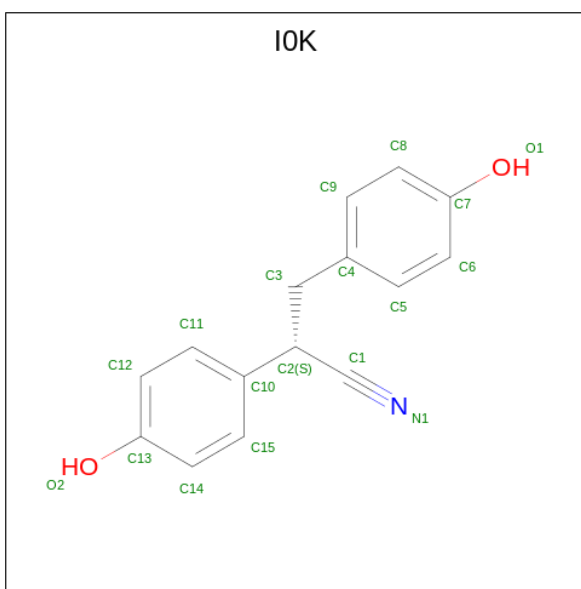
- Molecule 2 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	H	N	O	8	0	0
			177	54	93	14	16			
2	D	10	Total	C	H	N	O	6	0	0
			162	49	88	12	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	601	SER	GLN	conflict	UNP Q15788
C	602	GLY	THR	conflict	UNP Q15788
D	601	SER	GLN	conflict	UNP Q15788
D	602	GLY	THR	conflict	UNP Q15788

- Molecule 3 is (2 {S})-2,3-bis(4-hydroxyphenyl)propanenitrile (three-letter code: IOK) (formula: C₁₅H₁₃NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	2	0
			31	15	13	1	2		
3	B	1	Total	C	H	N	O	2	0
			31	15	13	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		

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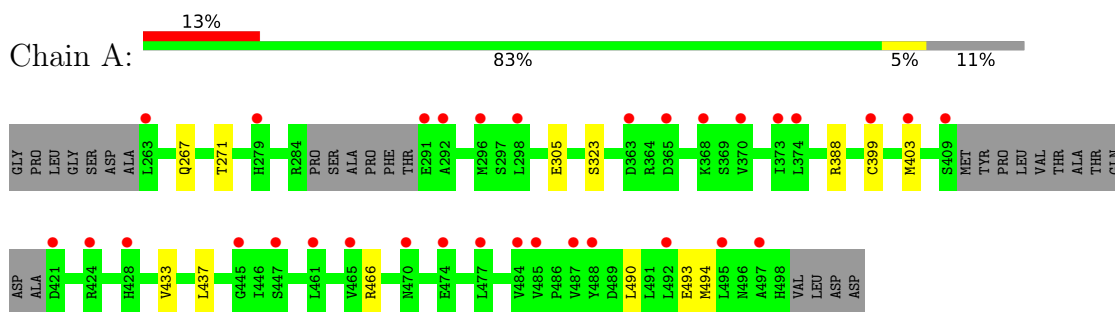
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	145	Total 145	O 145	0	0
4	C	8	Total 8	O 8	0	0
4	D	6	Total 6	O 6	0	0

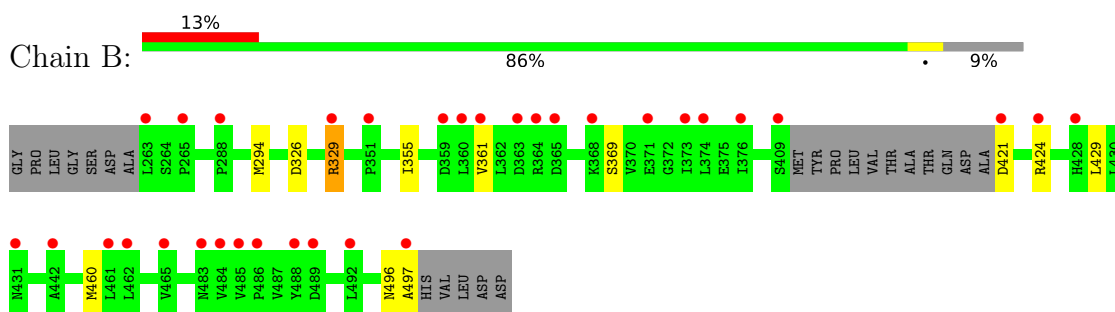
3 Residue-property plots [i](#)

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.

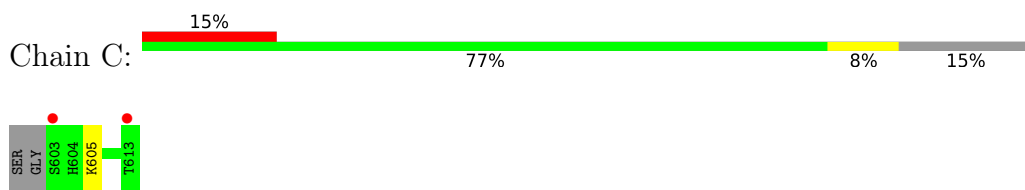
- Molecule 1: Estrogen receptor beta



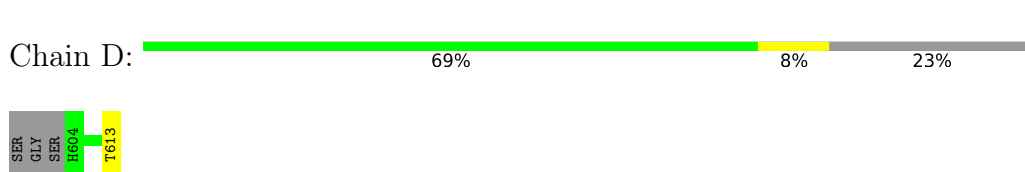
- Molecule 1: Estrogen receptor beta



- Molecule 2: Nuclear receptor coactivator 1



- Molecule 2: Nuclear receptor coactivator 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.19Å 89.01Å 101.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.44 – 1.54 46.40 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.44-1.54) 99.4 (46.40-1.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.55Å)	Xtrriage
Refinement program	REFMAC 5.8.0349	Depositor
R, R_{free}	0.206 , 0.237 0.217 , 0.247	Depositor DCC
R_{free} test set	3383 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtrriage
Anisotropy	0.038	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7668	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: I0K

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	0.61	3/1741 (0.2%)	0.83	0/2349
1	B	0.56	0/1746	0.84	1/2359 (0.0%)
2	C	0.48	0/84	0.95	0/112
2	D	0.43	0/73	0.97	0/99
All	All	0.58	3/3644 (0.1%)	0.84	1/4919 (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	2
1	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	SER	CA-CB	-5.41	1.44	1.52
1	A	493	GLU	CD-OE1	5.06	1.31	1.25
1	A	305	GLU	CD-OE2	-5.06	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	460	MET	CG-SD-CE	-7.92	87.52	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	388	ARG	Sidechain
1	A	466	ARG	Sidechain
1	B	329	ARG	Sidechain

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	1710	1769	1738	8	0
1	B	1716	1752	1706	8	0
2	C	84	93	91	1	0
2	D	74	88	85	1	0
3	A	18	13	0	0	0
3	B	18	13	0	0	0
4	A	161	0	0	0	0
4	B	145	0	0	1	0
4	C	8	0	0	1	0
4	D	6	0	0	1	0
All	All	3940	3728	3620	18	0

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 2.

All (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403[B]:MET:HE2	1:A:433:VAL:HG12	1.38	1.03
1:A:399:CYS:HB3	1:A:403[B]:MET:HE3	1.47	0.93
1:A:403[B]:MET:HE3	1:A:437:LEU:HB2	1.75	0.69
1:A:399:CYS:HB3	1:A:403[B]:MET:CE	2.21	0.68
1:B:429:LEU:CB	4:B:817:HOH:O	2.43	0.66
2:C:605:LYS:HE2	4:C:702:HOH:O	1.99	0.62
1:A:490:LEU:O	1:A:494[B]:MET:HG2	2.00	0.61
1:A:403[B]:MET:CE	1:A:437:LEU:HB2	2.35	0.57
1:B:496:ASN:O	1:B:497:ALA:HB2	2.08	0.54
2:D:613:THR:HG23	4:D:705:HOH:O	2.08	0.53
1:B:355:ILE:HD13	1:B:361:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLN:O	1:A:271:THR:HG23	2.11	0.51
1:B:496:ASN:O	1:B:497:ALA:CB	2.60	0.49
1:B:294[B]:MET:SD	1:B:369:SER:OG	2.71	0.49
1:B:421:ASP:HB3	1:B:424:ARG:NH1	2.31	0.46
1:B:326:ASP:OD1	1:B:329:ARG:NH1	2.52	0.42
1:B:355:ILE:CD1	1:B:361:VAL:HG13	2.48	0.42
1:A:403[B]:MET:HE1	1:A:433:VAL:O	2.20	0.41

There are no symmetry-related clashes.

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	217/247 (88%)	213 (98%)	4 (2%)	0	100	100
1	B	222/247 (90%)	217 (98%)	5 (2%)	0	100	100
2	C	9/13 (69%)	9 (100%)	0	0	100	100
2	D	8/13 (62%)	8 (100%)	0	0	100	100
All	All	456/520 (88%)	447 (98%)	9 (2%)	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	189/220 (86%)	189 (100%)	0	100	100
1	B	181/220 (82%)	181 (100%)	0	100	100
2	C	10/12 (83%)	10 (100%)	0	100	100
2	D	9/12 (75%)	9 (100%)	0	100	100
All	All	389/464 (84%)	389 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	478	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	I0K	A	601	-	19,19,19	0.33	0	23,25,25	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	I0K	B	601	-	19,19,19	0.45	0	23,25,25	0.69	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
3	I0K	A	601	-	-	0/8/10/10	0/2/2/2
3	I0K	B	601	-	-	0/8/10/10	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

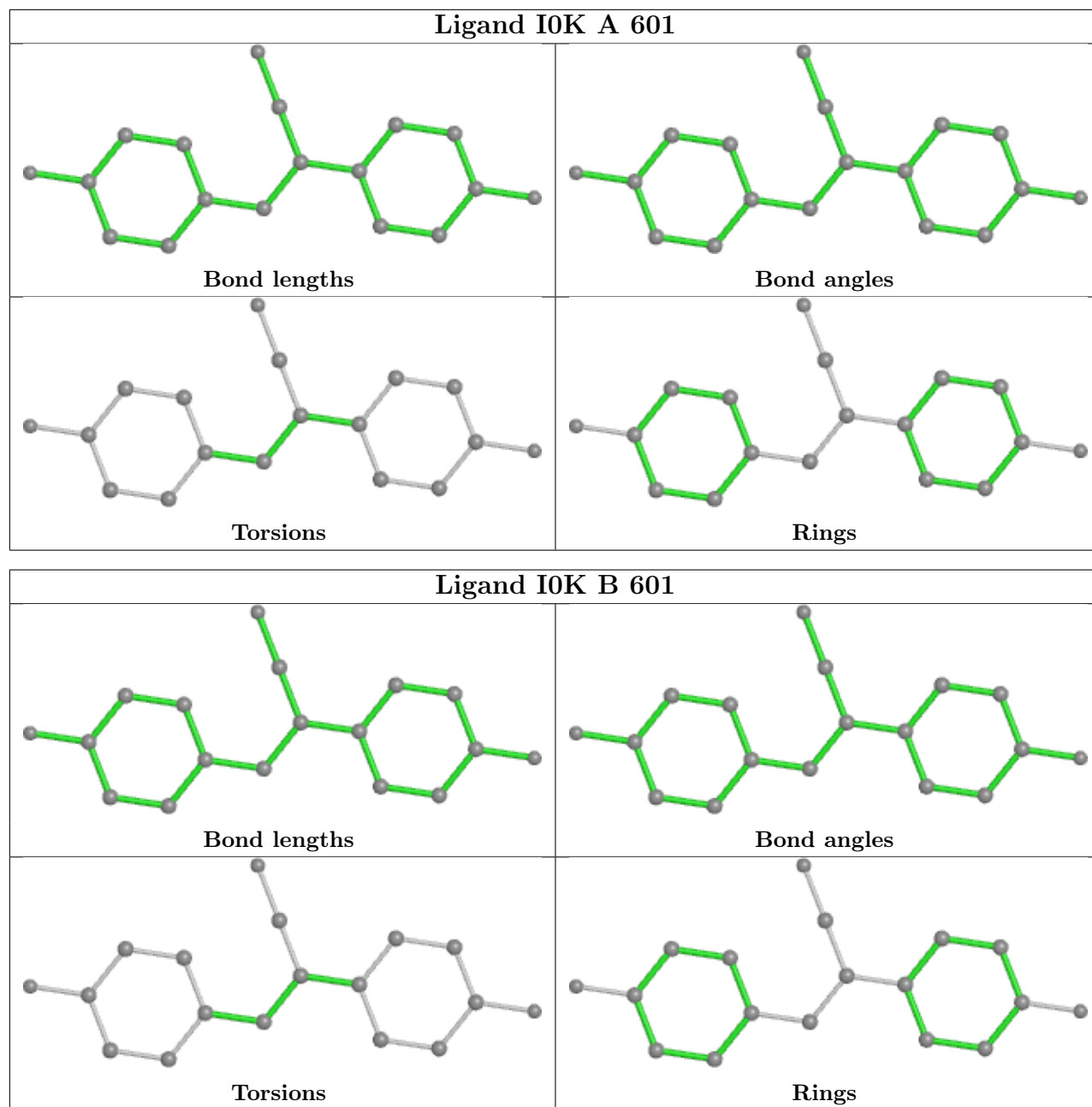
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/247 (88%)	1.32	32 (14%) 2 2	10, 21, 39, 56	0
1	B	224/247 (90%)	1.19	33 (14%) 2 2	10, 21, 41, 54	0
2	C	11/13 (84%)	1.55	2 (18%) 1 1	15, 23, 32, 45	0
2	D	10/13 (76%)	1.10	0 100 100	17, 20, 31, 33	0
All	All	464/520 (89%)	1.26	67 (14%) 2 2	10, 21, 41, 56	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	487	VAL	10.0
1	A	365	ASP	5.8
1	A	409	SER	5.4
1	B	263	LEU	5.2
1	B	492	LEU	5.2
1	A	485	VAL	4.8
2	C	613	THR	4.3
1	A	421	ASP	4.3
1	B	374	LEU	4.3
1	B	486	PRO	4.1
1	A	374	LEU	4.0
1	A	488	TYR	4.0
1	B	485	VAL	3.9
1	A	495	LEU	3.8
1	B	462	LEU	3.8
1	A	292	ALA	3.5
1	A	424	ARG	3.5
1	A	497	ALA	3.4
1	B	484	VAL	3.3
1	A	484	VAL	3.3
1	A	263	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	447	SER	3.2
1	B	424	ARG	3.2
1	B	488	TYR	3.1
1	B	497	ALA	3.0
1	B	363	ASP	3.0
1	A	291	GLU	3.0
1	B	365	ASP	2.9
1	A	445	GLY	2.8
1	A	279	HIS	2.8
1	B	329	ARG	2.8
1	B	359	ASP	2.8
1	A	403[A]	MET	2.8
1	B	361	VAL	2.7
1	B	351	PRO	2.7
1	B	368	LYS	2.7
1	B	428	HIS	2.6
1	B	461	LEU	2.6
1	A	370	VAL	2.6
1	B	483	ASN	2.6
1	B	371	GLU	2.6
1	B	421	ASP	2.6
1	A	296	MET	2.5
1	A	298	LEU	2.5
1	A	461	LEU	2.5
1	B	409	SER	2.5
1	A	373	ILE	2.5
1	A	465	VAL	2.4
1	B	376	ILE	2.4
1	A	363	ASP	2.4
1	B	442	ALA	2.3
1	A	474	GLU	2.3
1	A	368	LYS	2.3
1	B	360	LEU	2.2
1	B	288	PRO	2.2
1	A	477	LEU	2.2
1	B	489	ASP	2.2
2	C	603	SER	2.2
1	A	470	ASN	2.2
1	B	364	ARG	2.1
1	A	428	HIS	2.1
1	A	399	CYS	2.1
1	B	431[A]	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	492	LEU	2.1
1	B	373	ILE	2.0
1	B	465	VAL	2.0
1	B	265	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

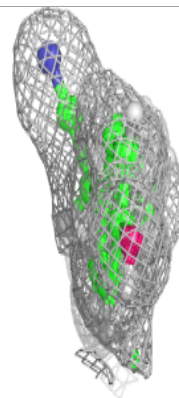
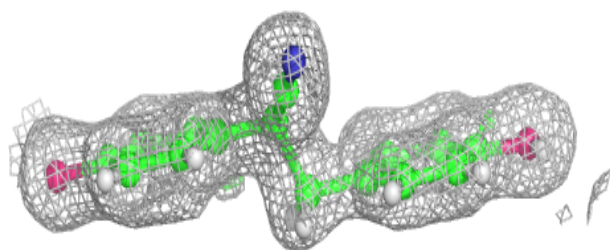
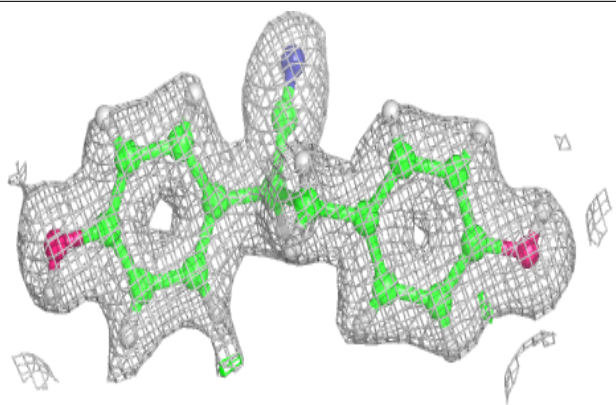
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	I0K	B	601	18/18	0.94	0.12	13,15,19,21	2
3	I0K	A	601	18/18	0.96	0.12	13,16,19,20	2

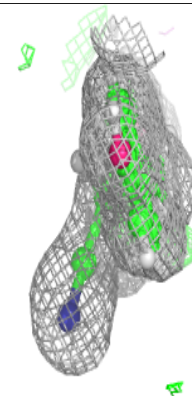
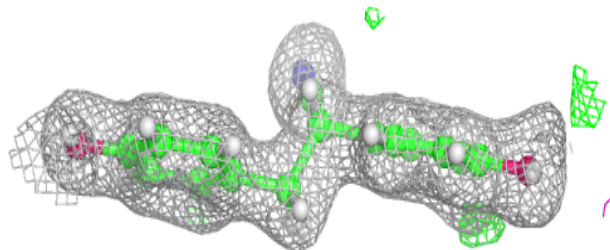
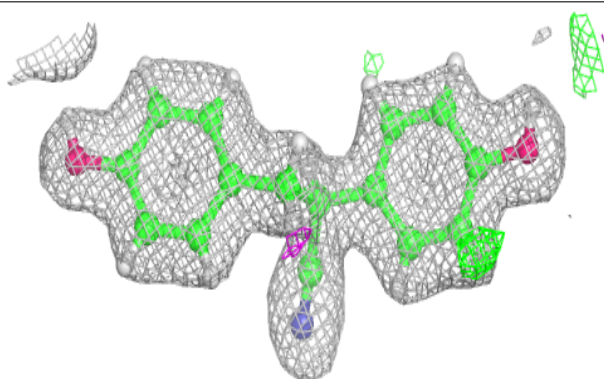
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around I0K 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 I0K A 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.