Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 08:50 PM JST

PDB ID	:	7DHL
Title	:	Crystal structure of FGFR3 in complex with pyrimidine derivative
Authors	:	Echizen, Y.; Tateishi, Y.; Amano, Y.
Deposited on	:	2020-11-16
Resolution	:	2.57 Å(reported)

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

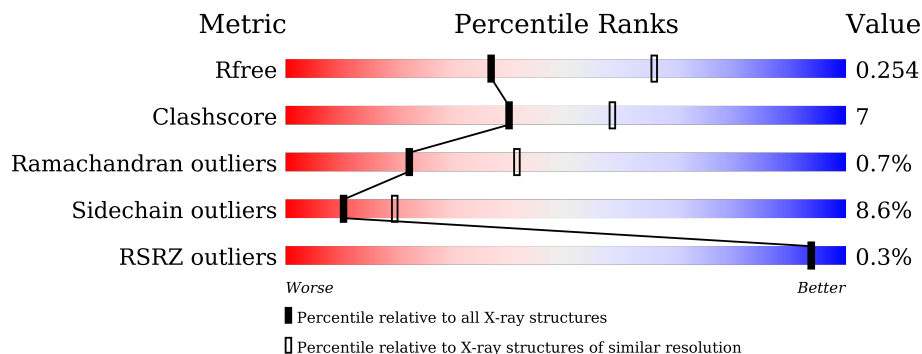|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.57 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		0.254
Clashscore		7
Ramachandran outliers		0.7%
Sidechain outliers		8.6%
RSRZ outliers		0.3%

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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	313	73% 16% • 8%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 2361 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 Fibroblast growth factor receptor 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	289	2307	1469	392	425	3	18	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	GLY	-	expression tag	UNP P22607
A	448	SER	-	expression tag	UNP P22607
A	449	HIS	-	expression tag	UNP P22607
A	450	MET	-	expression tag	UNP P22607
A	451	LEU	-	expression tag	UNP P22607
A	452	ALA	-	expression tag	UNP P22607
A	453	GLY	-	expression tag	UNP P22607
A	454	VAL	-	expression tag	UNP P22607
A	455	SER	-	expression tag	UNP P22607
A	456	GLU	-	expression tag	UNP P22607
A	457	TYR	-	expression tag	UNP P22607
A	458	GLU	-	expression tag	UNP P22607
A	459	LEU	-	expression tag	UNP P22607
A	460	PRO	-	expression tag	UNP P22607
A	461	GLU	-	expression tag	UNP P22607
A	462	ASP	-	expression tag	UNP P22607
A	463	PRO	-	expression tag	UNP P22607
A	464	LYS	-	expression tag	UNP P22607
A	465	TRP	-	expression tag	UNP P22607
A	466	GLU	-	expression tag	UNP P22607
A	467	PHE	-	expression tag	UNP P22607
A	468	PRO	-	expression tag	UNP P22607
A	469	ARG	-	expression tag	UNP P22607
A	470	ASP	-	expression tag	UNP P22607
A	471	LYS	-	expression tag	UNP P22607

- Molecule 2 is 5-[2-(3,5-dimethoxyphenyl)ethyl]-N-[3-methoxy-4-[4-(4-methylpiperazin-1-yl

)piperidin-1-yl]phenyl]pyrimidin-2-amine (three-letter code: H6X) (formula: $C_{31}H_{42}N_6O_3$) (labeled as "Ligand of Interest" by depositor).
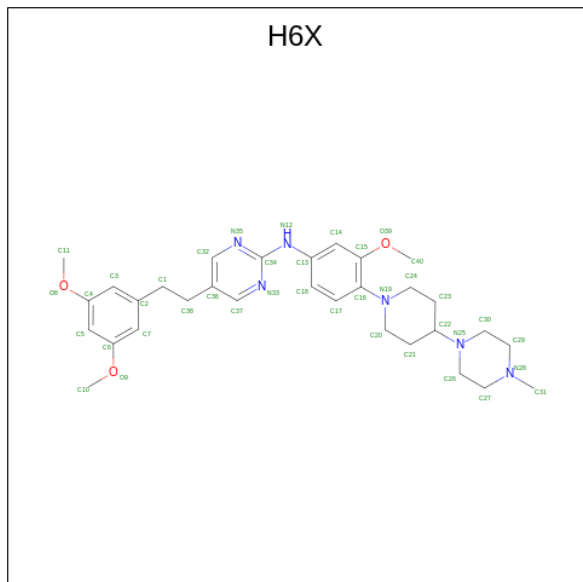
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	40	31	6	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	14	14	14	0	0

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: Fibroblast growth factor receptor 3
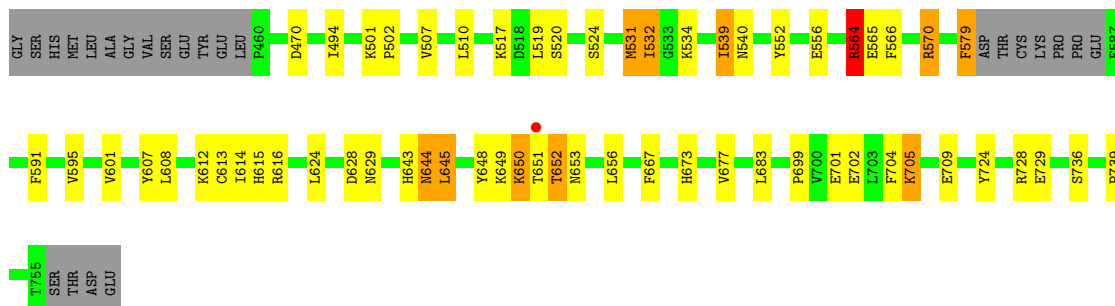
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.14Å 61.40Å 59.90Å 90.00° 112.88° 90.00°	Depositor
Resolution (Å)	44.35 – 2.57 44.35 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.35-2.57) 99.4 (44.35-2.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.193 , 0.254 0.194 , 0.254	Depositor DCC
R_{free} test set	484 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2361	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: PTR, H6X

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	0.32	0/2306	0.69	1/3112 (0.0%)

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	564	ARG	CG-CD-NE	6.24	124.89	111.80

There are no chirality outliers.

There are no planarity outliers.

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	2307	0	2297	33	0
2	A	40	0	0	1	0
3	A	14	0	0	0	0
All	All	2361	0	2297	34	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 7.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:PTR:O1P	1:A:650:LYS:HE3	1.75	0.86
1:A:729:GLU:HG3	1:A:739:PRO:HD3	1.62	0.80
1:A:645:LEU:H	1:A:645:LEU:HD12	1.45	0.80
1:A:614:ILE:HG22	1:A:616:ARG:HG3	1.63	0.79
1:A:644:ASN:HD22	1:A:644:ASN:H	1.36	0.72
1:A:532:ILE:HD13	1:A:608:LEU:HD11	1.78	0.65
1:A:564:ARG:HH11	1:A:564:ARG:HG2	1.60	0.65
1:A:644:ASN:H	1:A:644:ASN:ND2	2.01	0.57
1:A:644:ASN:ND2	1:A:644:ASN:N	2.55	0.54
1:A:566:PHE:O	1:A:570:ARG:HD2	2.09	0.53
1:A:510:LEU:HD11	1:A:519:LEU:HD13	1.90	0.51
1:A:601:VAL:HG11	1:A:683:LEU:CD2	2.41	0.51
1:A:667:PHE:HE1	1:A:704:PHE:CD1	2.29	0.51
1:A:724:TYR:CZ	1:A:728:ARG:HD3	2.45	0.51
1:A:615:HIS:O	1:A:616:ARG:HB2	2.12	0.49
1:A:539:ILE:HD13	1:A:624:LEU:HD12	1.95	0.49
1:A:507:VAL:CG1	1:A:552:TYR:HB3	2.42	0.49
1:A:612:LYS:HD3	1:A:643:HIS:ND1	2.28	0.48
1:A:699:PRO:HB2	1:A:701:GLU:OE2	2.13	0.48
2:A:801:H6X:N33	2:A:801:H6X:C14	2.76	0.47
1:A:579:PHE:CD1	1:A:579:PHE:N	2.84	0.45
1:A:628:ASP:O	1:A:629:ASN:HB2	2.16	0.45
1:A:564:ARG:NH1	1:A:565:GLU:OE2	2.50	0.44
1:A:520:SER:O	1:A:524:SER:HB2	2.17	0.44
1:A:540:ASN:N	1:A:556:GLU:OE1	2.47	0.43
1:A:705:LYS:O	1:A:709:GLU:HG3	2.17	0.43
1:A:729:GLU:CG	1:A:739:PRO:HD3	2.42	0.43
1:A:673:HIS:O	1:A:677:VAL:HG23	2.19	0.43
1:A:591:PHE:O	1:A:595:VAL:HG23	2.18	0.42
1:A:501:LYS:HA	1:A:502:PRO:HD3	1.89	0.41
1:A:539:ILE:HG13	1:A:556:GLU:HG3	2.03	0.41
1:A:540:ASN:H	1:A:556:GLU:CG	2.33	0.41
1:A:532:ILE:O	1:A:607:TYR:OH	2.32	0.40
1:A:650:LYS:C	1:A:652:THR:H	2.24	0.40

There are no symmetry-related clashes.

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	282/313 (90%)	270 (96%)	10 (4%)	2 (1%)	22	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	531	MET
1	A	532	ILE

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	244/266 (92%)	223 (91%)	21 (9%)	10	19

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	470	ASP
1	A	494	ILE
1	A	517	LYS
1	A	531	MET
1	A	534	LYS
1	A	539	ILE
1	A	564	ARG
1	A	570	ARG
1	A	579	PHE

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Mol	Chain	Res	Type
1	A	613	CYS
1	A	644	ASN
1	A	645	LEU
1	A	649	LYS
1	A	650	LYS
1	A	651	THR
1	A	652	THR
1	A	653	ASN
1	A	656	LEU
1	A	702	GLU
1	A	705	LYS
1	A	736	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	540	ASN
1	A	588	GLN
1	A	622	ASN
1	A	644	ASN
1	A	653	ASN
1	A	718	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	PTR	A	577	1	15,16,17	0.44	0	19,22,24	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	PTR	A	648	1	15,16,17	0.51	0	19,22,24	0.89	0
1	PTR	A	647	1	15,16,17	0.43	0	19,22,24	0.57	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	PTR	A	577	1	-	1/10/11/13	0/1/1/1
1	PTR	A	648	1	-	2/10/11/13	0/1/1/1
1	PTR	A	647	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	577	PTR	CZ-OH-P-O1P
1	A	648	PTR	C-CA-CB-CG
1	A	648	PTR	CE2-CZ-OH-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	648	PTR	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	H6X	A	801	-	44,44,44	1.22	5 (11%)	59,60,60	2.26	19 (32%)

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	H6X	A	801	-	-	9/23/43/43	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	H6X	C26-N25	2.98	1.52	1.47
2	A	801	H6X	C30-N25	2.96	1.52	1.47
2	A	801	H6X	C27-N28	2.74	1.52	1.46
2	A	801	H6X	C29-N28	2.73	1.52	1.46
2	A	801	H6X	C34-N12	2.32	1.41	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
2	A	801	H6X	C40-O39-C15	-5.83	108.73	117.53
2	A	801	H6X	O39-C15-C14	-5.13	115.28	124.12
2	A	801	H6X	O39-C15-C16	5.10	123.02	116.06
2	A	801	H6X	C29-N28-C27	4.99	116.50	109.52
2	A	801	H6X	C17-C16-N19	-4.27	115.49	122.30
2	A	801	H6X	C30-N25-C26	3.83	116.08	109.08
2	A	801	H6X	C10-O9-C6	-3.52	109.86	117.51
2	A	801	H6X	C15-C16-N19	3.41	125.69	119.33
2	A	801	H6X	C31-N28-C27	3.37	115.70	110.66
2	A	801	H6X	N35-C34-N33	-3.31	122.95	126.43
2	A	801	H6X	C38-C36-C37	3.28	127.12	121.83
2	A	801	H6X	C11-O8-C4	-3.11	110.77	117.51
2	A	801	H6X	C24-N19-C20	3.09	118.33	111.52
2	A	801	H6X	C31-N28-C29	2.97	115.11	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	H6X	C38-C36-C32	-2.70	117.47	121.83
2	A	801	H6X	C30-N25-C22	2.60	119.95	112.64
2	A	801	H6X	C30-C29-N28	2.56	113.70	110.80
2	A	801	H6X	C24-N19-C16	2.46	122.09	116.27
2	A	801	H6X	N12-C34-N33	2.23	123.19	116.28

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	H6X	C15-C16-N19-C24
2	A	801	H6X	C21-C22-N25-C30
2	A	801	H6X	C23-C22-N25-C30
2	A	801	H6X	C17-C16-N19-C24
2	A	801	H6X	C23-C22-N25-C26
2	A	801	H6X	C16-C15-O39-C40
2	A	801	H6X	C14-C15-O39-C40
2	A	801	H6X	C21-C22-N25-C26
2	A	801	H6X	C15-C16-N19-C20

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	H6X	1	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 H6X A 801

Bond lengths

Bond angles

Torsions

Rings
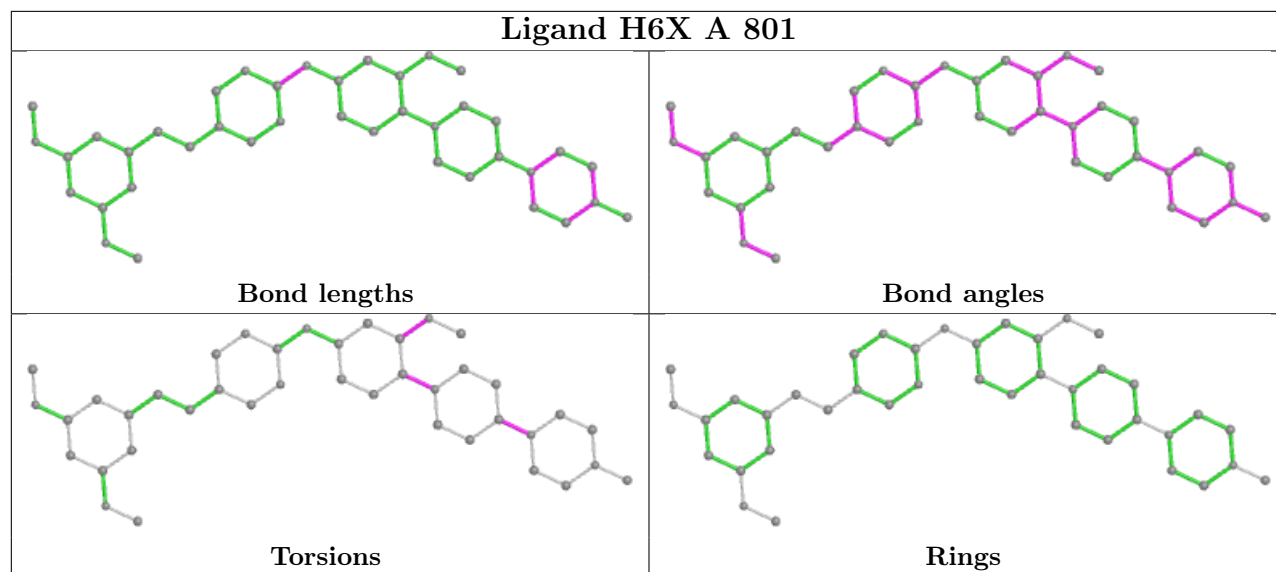
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	286/313 (91%)	-0.03	1 (0%)	94	94	28, 46, 82, 108	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	651	THR	2.1

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.

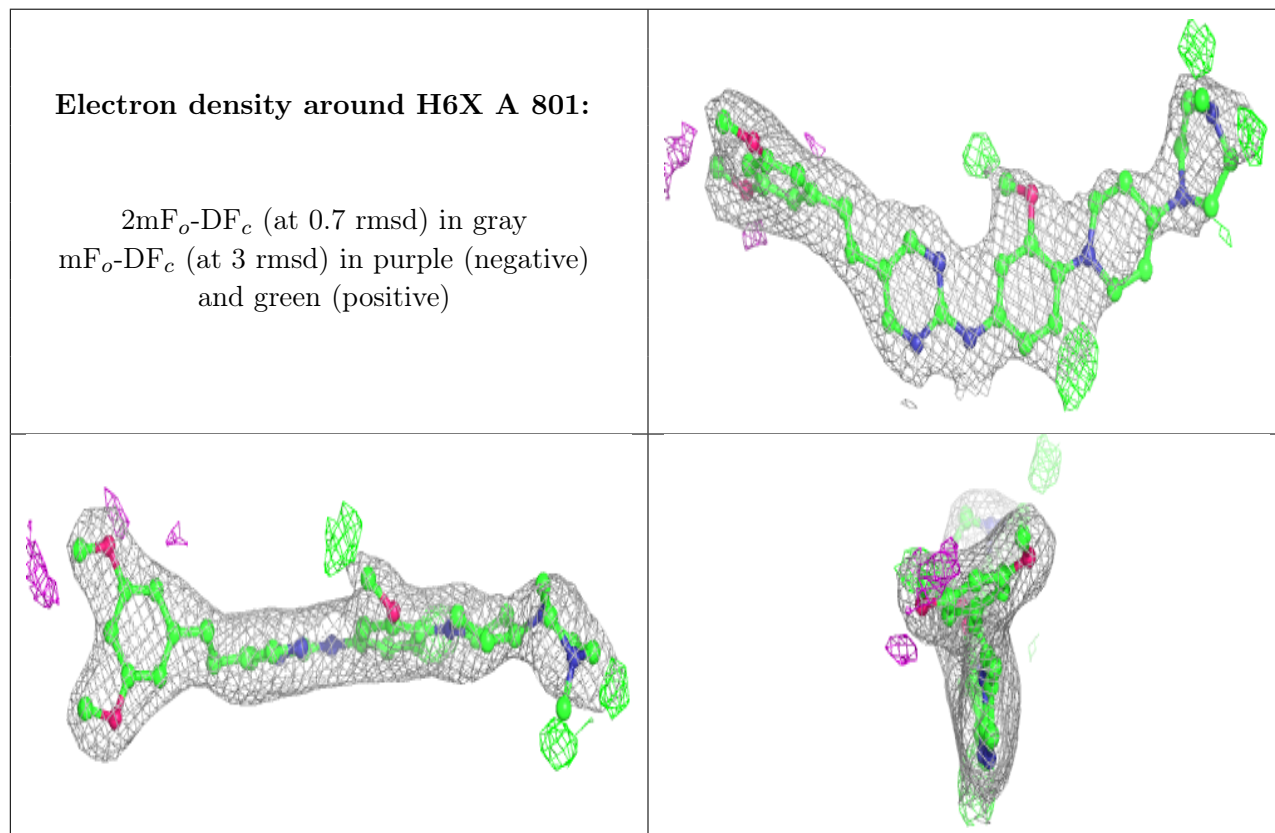| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	PTR	A	577	16/17	0.89	0.18	68,81,113,118	0
1	PTR	A	647	16/17	0.92	0.16	64,70,83,87	0
1	PTR	A	648	16/17	0.97	0.14	49,52,62,67	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	H6X	A	801	40/40	0.94	0.16	30,49,99,102	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 H6X A 801:

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

6.5 Other polymers (i)

There are no such residues in this entry.