

wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 04:18 am BST

PDB ID : 3ZLQ

Title : BACE2 XAPERONE COMPLEX

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Deposited on : 2013-02-04

Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The 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 : 2.11

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)

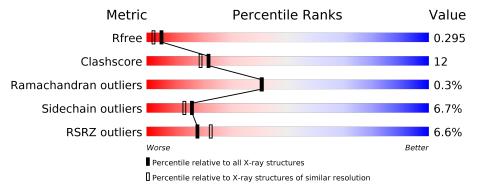
Validation Pipeline (wwPDB-VP) : 2.11

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 2.10 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range}(ext{Å})) \end{aligned}$		
R_{free}	130704	5197 (2.10-2.10)		
Clashscore	141614	5710 (2.10-2.10)		
Ramachandran outliers	138981	5647 (2.10-2.10)		
Sidechain outliers	138945	5648 (2.10-2.10)		
RSRZ outliers	127900	5083 (2.10-2.10)		

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 on 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	386	66%	27%	• 5%				
1	В	386	11% 72%	21%					
2	С	122	70%	21%	8%				
2	D	122	68%	23%	• 8%				



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7613 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 BETA-SECRETASE 2.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Δ	367	10001	С	11	О	S	0	1	0
1		307	2843	1827	455	548	13			
1	D	370	Total	С	N	О	S	0	9	0
1	Б	370	2878	1854	459	552	13	0	<u> </u>	

There are 2 discrepancies between the modelled and reference sequences:

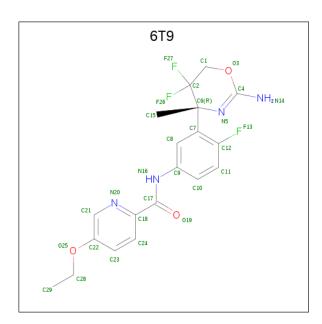
Chain	Residue	Modelled	Actual	Comment	Reference
A	269	ALA	GLU	engineered mutation	UNP Q9Y5Z0
В	269	ALA	GLU	engineered mutation	UNP Q9Y5Z0

• Molecule 2 is a protein called XA4813.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	С	112	Total	otal C N O S	0	0				
2		112	833	512	151	166	4	0	U	
9	D	112	Total	С	N	О	S	0	1	0
	D	112	842	517	153	168	4	0		

• Molecule 3 is 5-Ethoxy-pyridine-2-carboxylic acid [3-((R)-2-amino-5,5-difluoro-4-methyl-5,6-dihydro-4H-[1,3]oxazin-4-yl)-4-fluoro-phenyl]-amide (three-letter code: 6T9) (formula: C₁₉H₁₉F₃N₄O₃).





Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf		
9	Λ	1	Total	С	F	N	О	0	0	
$\begin{array}{c c} & A \\ \end{array}$	1	29	19	3	4	3	0			
9	D	1	Total	С	F	N	О	0	0	
ა	Б	1	29	19	3	4	3	U		

• Molecule 4 is water.

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	${f AltConf}$
4	A	74	Total O 74 74	0	0
4	В	51	Total O 51 51	0	0
4	С	16	Total O 16 16	0	0
4	D	18	Total O 18 18	0	0

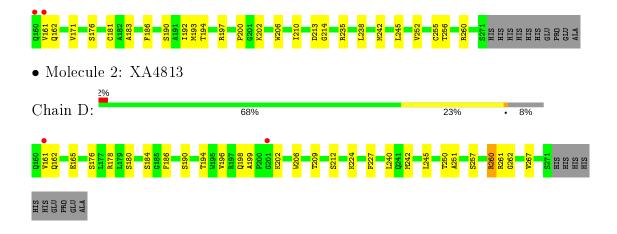


3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: BETA-SECRETASE 2







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	46.78Å 210.98Å 53.30Å	Depositor
a, b, c, α , β , γ	90.00° 105.07° 90.00°	Depositor
Resolution (Å)	46.26 - 2.10	Depositor
resolution (A)	46.26 - 2.10	EDS
% Data completeness	88.6 (46.26-2.10)	Depositor
(in resolution range)	88.6 (46.26-2.10)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.44 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
P. P.	0.238 , 0.296	Depositor
R, R_{free}	0.236 , 0.295	DCC
R_{free} test set	2596 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 39.4	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7613	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 19.03% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: 6T9

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	Boı	nd lengths	Bond angles		
MIOI		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.88	$1/2912 \ (0.0\%)$	0.97	$7/3959 \ (0.2\%)$	
1	В	0.77	$1/2948 \ (0.0\%)$	0.92	1/4008~(0.0%)	
2	С	0.80	0/847	1.00	3/1146 (0.3%)	
2	D	0.86	0/856	0.93	0/1158	
All	All	0.83	$2/7563 \ (0.0\%)$	0.95	11/10271 (0.1%)	

All (2) bond length outliers are listed below:

Mol	Chain	${f Res}$	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
1	В	92	TRP	CB-CG	6.83	1.62	1.50
1	A	92	TRP	CB-CG	6.41	1.61	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
1	A	310	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	A	86	LYS	CB-CA-C	-6.19	98.03	110.40
2	С	193	MET	CG-SD-CE	6.17	110.06	100.20
1	A	310	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	28	ARG	NE-CZ-NH1	6.08	123.34	120.30

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



D

All

18

7613

4

All

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2843	0	2757	73	0
1	В	2878	0	2798	69	1
2	С	833	0	814	14	0
2	D	842	0	821	19	0
3	A	29	0	19	3	0
3	В	29	0	19	4	0
4	A	74	0	0	7	0
4	В	51	0	0	4	0
4	С	16	0	0	0	0

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

0

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 12.

0

7228

 $\overline{2}$

174

0

1

The worst 5 of 174 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap} & (ext{Å}) \end{aligned}$
1:B:79:LYS:HE2	2:D:190:SER:O	1.59	1.00
3:A:1398:6T9:O19	3:A:1398:6T9:H10	1.71	0.90
2:D:198:GLN:HG2	4:D:2006:HOH:O	1.75	0.84
1:B:26:SER:HB3	1:B:351:GLU:OE2	1.77	0.84
1:A:64:ILE:HG22	4:A:2015:HOH:O	1.82	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{array}{l} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:B:120:GLU:OE2	1:B:363:ARG:NH2[1_455]	2.10	0.10

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	Perce	entiles
1	A	$362/386 \; (94\%)$	338 (93%)	23 (6%)	1 (0%)	41	41
1	В	$366/386 \; (95\%)$	343 (94%)	21 (6%)	2 (0%)	29	26
2	С	110/122~(90%)	105 (96%)	5 (4%)	0	100	100
2	D	111/122 (91%)	106 (96%)	5 (4%)	0	100	100
All	All	949/1016 (93%)	892 (94%)	54 (6%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ALA
1	В	265	SER
1	В	288	THR

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	Percer	$_{ m ntiles}$
1	A	307/319 (96%)	285 (93%)	22 (7%)	14	11
1	В	311/319 (98%)	292 (94%)	19 (6%)	18	16
2	С	90/99 (91%)	84 (93%)	6 (7%)	16	13
2	D	91/99 (92%)	84 (92%)	7 (8%)	13	9
All	All	799/836~(96%)	745 (93%)	54 (7%)	16	13

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	102	THR
1	В	286	SER
2	D	176	SER
1	В	108	ASN
1	В	219	LEU



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	A	108	ASN
1	В	108	ASN
1	В	224	GLN

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 carbohydrates 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	Tuno	Chain	Res	Link	Bo	ond leng	an	B	ond ang	gles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6T9	A	1398	-	29,31,31	1.25	3 (10%)	36,46,46	2.24	13 (36%)
3	6T9	В	1398	-	29,31,31	1.03	2 (6%)	36,46,46	1.88	10 (27%)

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	6T9	A	1398	-	-	3/16/37/37	0/3/3/3
3	6T9	В	1398	-	-	2/16/37/37	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
3	В	1398	6T9	C8-C7	-3.36	1.34	1.39
3	A	1398	6T9	C1-C2	2.52	1.56	1.52
3	A	1398	6T9	C8-C7	-2.35	1.35	1.39
3	В	1398	6T9	C21-N20	-2.20	1.29	1.34
3	A	1398	6T9	O19-C17	-2.10	1.19	1.23

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	1398	6T9	F27-C2-F26	7.42	113.95	104.93
3	В	1398	6T9	C15-C6-N5	4.80	113.57	108.81
3	A	1398	6T9	C22-C21-N20	-4.63	117.28	122.73
3	В	1398	6T9	C21-N20-C18	3.75	123.19	117.36
3	A	1398	6T9	C9-N16-C17	-3.67	117.06	126.58

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1398	6T9	C29-C28-O25-C22
3	В	1398	6T9	C29-C28-O25-C22
3	A	1398	6T9	C23-C22-O25-C28
3	A	1398	6T9	C15-C6-C7-C8
3	В	1398	6T9	C15-C6-C7-C8

There are no ring outliers.

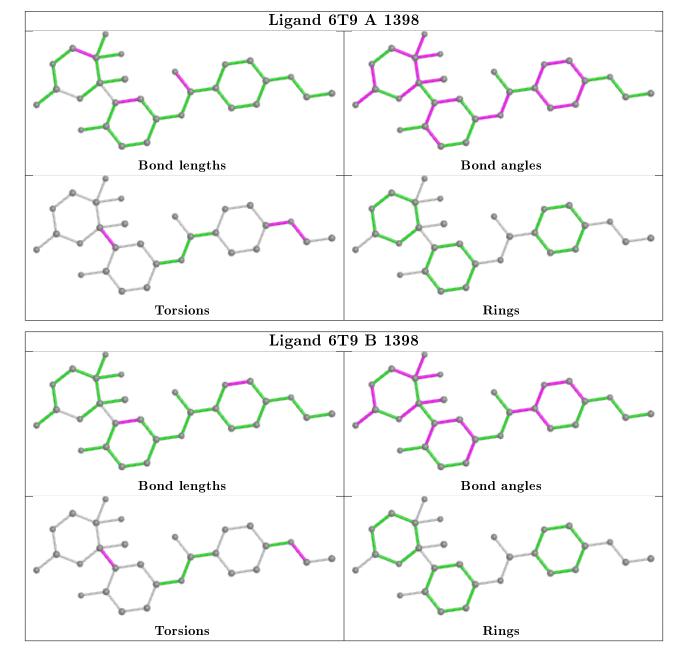
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1398	6T9	3	0
3	В	1398	6T9	4	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.



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	$367/386 \; (95\%)$	0.46	16 (4%) 34 40	15, 26, 48, 58	11 (2%)
1	В	370/386~(95%)	0.75	43 (11%) 4 6	16, 30, 60, 85	12 (3%)
2	С	112/122 (91%)	0.28	2 (1%) 68 72	16, 25, 42, 66	3 (2%)
2	D	112/122 (91%)	0.18	2 (1%) 68 72	16, 25, 40, 57	1 (0%)
All	All	961/1016 (94%)	0.52	63 (6%) 18 23	15, 27, 53, 85	27 (2%)

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	88	THR	5.2
1	A	227	ASN	4.9
1	A	88	THR	4.7
1	В	227	ASN	4.6
1	В	390	ASP	4.3

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 carbohydrates in this entry.

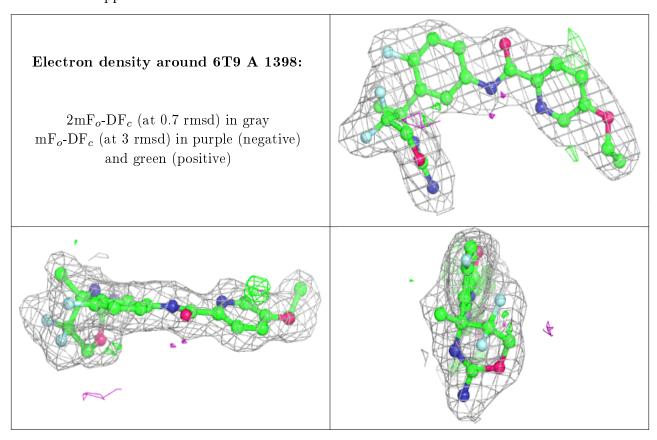
6.4 Ligands (i)

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

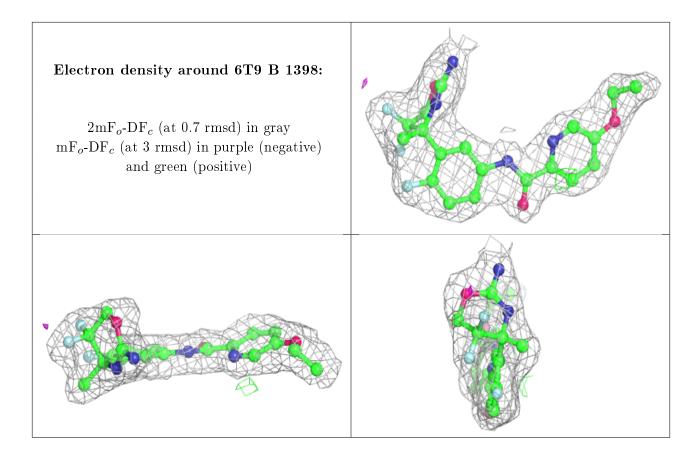


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$ m ig B ext{-factors}(\AA^2)$	Q<0.9
3	6T9	A	1398	29/29	0.93	0.14	19,24,27,30	0
3	6T9	В	1398	29/29	0.93	0.14	24,26,31,33	0

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.







6.5 Other polymers (i)

There are no such residues in this entry.

