



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:42 PM UTC

PDB ID : 5QDA / pdb_00005qda
Title : Crystal structure of BACE complex with BMC013
Authors : Rondeau, J.M.; Shao, C.; Yang, H.; Burley, S.K.
Deposited on : 2017-12-01
Resolution : 2.10 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

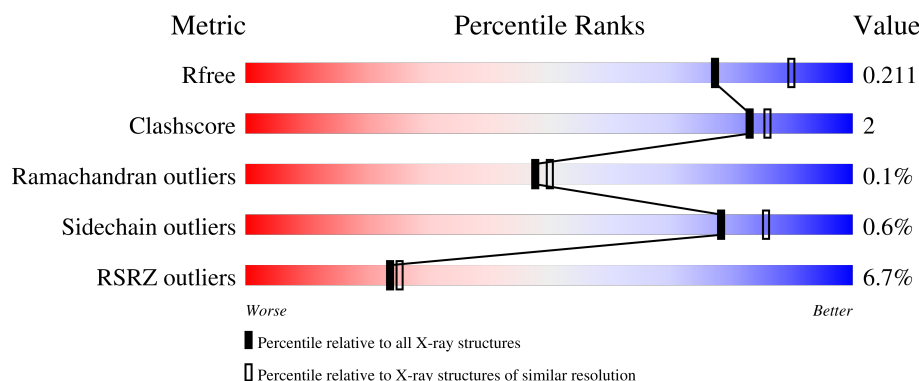
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	402	6% 86% 7% 6%
1	B	402	7% 88% 5% 6%
1	C	402	6% 88% 7% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9384 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.

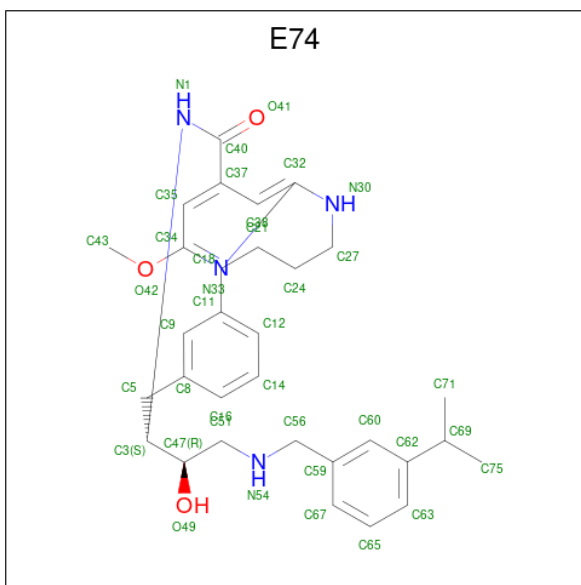
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	B	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	C	381	Total	C	N	O	S	0	0	0
			2993	1917	497	565	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	expression tag	UNP P56817
A	-14	PRO	-	expression tag	UNP P56817
B	-15	GLY	-	expression tag	UNP P56817
B	-14	PRO	-	expression tag	UNP P56817
C	-15	GLY	-	expression tag	UNP P56817
C	-14	PRO	-	expression tag	UNP P56817

- Molecule 2 is (4S)-4-[(1R)-1-hydroxy-2-({3-(propan-2-yl)phenyl}methyl)amino]ethyl]-18-methoxy-3,15,17-triazatricyclo[14.3.1.1^{6,10}]henicosa-1(20),6(21),7,9,16,18-hexaen-2-one (CCD ID: E74) (formula: C₃₁H₄₀N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 38	C 31	N 4	O 3	0	0
2	B	1	Total 38	C 31	N 4	O 3	0	0
2	C	1	Total 38	C 31	N 4	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	118	Total O 118 118	0	0
3	B	93	Total O 93 93	0	0
3	C	134	Total O 134 134	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.60Å 104.06Å 100.05Å 90.00° 104.66° 90.00°	Depositor
Resolution (Å)	41.99 – 2.10 41.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.99-2.10) 97.9 (41.99-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.12_2829, CNX	Depositor
R, R_{free}	0.181 , 0.209 0.183 , 0.211	Depositor DCC
R_{free} test set	4692 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9384	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: E74

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	0/3041	0.54	0/4133
1	B	0.32	0/3041	0.54	0/4133
1	C	0.32	0/3070	0.55	0/4173
All	All	0.32	0/9152	0.55	0/12439

There are no bond length outliers.

There are no bond angle outliers.

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	2966	0	2878	17	0
1	B	2966	0	2878	10	0
1	C	2993	0	2902	17	0
2	A	38	0	0	0	0
2	B	38	0	0	0	0
2	C	38	0	0	0	0
3	A	118	0	0	0	0
3	B	93	0	0	1	0
3	C	134	0	0	4	0
All	All	9384	0	8658	43	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 (43) 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:205:ARG:NH1	3:B:501:HOH:O	2.12	0.82
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.81	0.62
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.84	0.60
1:A:301:LEU:HD12	1:A:361:VAL:HG23	1.86	0.58
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.85	0.58
1:C:75:LYS:NZ	3:C:503:HOH:O	2.36	0.58
1:B:215:MET:HE3	1:B:239:LYS:HE3	1.85	0.57
1:C:378:ASP:HB2	3:C:586:HOH:O	2.06	0.56
1:C:202:ILE:CD1	1:C:379:MET:HG3	2.37	0.54
1:C:288:MET:HE1	1:C:379:MET:HE3	1.89	0.54
1:C:13:GLY:HA3	1:C:30:LEU:HD11	1.91	0.52
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.91	0.52
1:B:125:GLU:CD	1:B:195:ARG:HH21	2.17	0.52
1:A:235:ARG:HB2	1:A:332:VAL:HB	1.93	0.50
1:A:311:ASP:HB2	1:A:319:CYS:SG	2.52	0.50
1:A:254:THR:HG21	1:C:254:THR:HG21	1.94	0.49
1:C:114:ASN:N	3:C:501:HOH:O	1.97	0.48
1:B:20:VAL:HG12	1:B:85:VAL:HG22	1.94	0.48
1:A:272:ALA:HB2	1:A:316:GLN:O	2.13	0.48
1:C:197:TRP:CG	1:C:198:TYR:H	2.32	0.47
1:C:54:ARG:NH1	1:C:79:GLU:OE1	2.34	0.47
1:A:267:LEU:HD12	1:A:319:CYS:HB3	1.95	0.47
1:C:335:ALA:O	1:C:339:GLU:HG3	2.15	0.47
1:B:197:TRP:CG	1:B:198:TYR:H	2.33	0.47
1:A:198:TYR:CE2	1:A:224:LYS:HE3	2.49	0.46
1:C:301:LEU:HD12	1:C:361:VAL:HG23	1.97	0.46
1:A:197:TRP:CG	1:A:198:TYR:H	2.34	0.46
1:B:340:GLY:HA2	1:B:360:HIS:HA	1.96	0.46
1:C:222:TYR:HA	1:C:223:ASP:HA	1.69	0.46
1:A:222:TYR:HA	1:A:223:ASP:HA	1.62	0.46
1:C:304:GLN:HG3	1:C:361:VAL:HG11	1.98	0.45
1:A:154:LEU:O	1:A:339:GLU:HA	2.16	0.45
1:A:13:GLY:HA3	1:A:30:LEU:HD11	1.99	0.45
1:C:202:ILE:HD11	1:C:379:MET:HG3	1.98	0.45
1:B:9:LYS:HA	1:B:169:SER:HB3	2.00	0.44
1:B:222:TYR:HA	1:B:223:ASP:HA	1.66	0.43
1:C:114:ASN:HA	3:C:501:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LEU:HD12	1:B:319:CYS:HB3	2.01	0.42
1:A:276:PRO:O	1:A:279:ILE:HG12	2.19	0.42
1:A:335:ALA:O	1:A:339:GLU:HG3	2.20	0.42
1:C:235:ARG:HB3	1:C:327:SER:HB2	2.02	0.41
1:A:363:ASP:HB3	1:A:366:ARG:O	2.21	0.41
1:A:95:VAL:HG11	1:A:140:LEU:HA	2.02	0.40

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	373/402 (93%)	361 (97%)	12 (3%)	0	100	100
1	B	373/402 (93%)	358 (96%)	14 (4%)	1 (0%)	36	36
1	C	377/402 (94%)	364 (97%)	13 (3%)	0	100	100
All	All	1123/1206 (93%)	1083 (96%)	39 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	PRO

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	322/342 (94%)	322 (100%)	0	100	100
1	B	322/342 (94%)	319 (99%)	3 (1%)	70	78
1	C	324/342 (95%)	321 (99%)	3 (1%)	70	78
All	All	968/1026 (94%)	962 (99%)	6 (1%)	78	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	TRP
1	B	325	SER
1	B	361	VAL
1	C	267	LEU
1	C	325	SER
1	C	362	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	278	ASN
1	B	53	GLN
1	B	89	HIS
1	B	211	GLN
1	B	271	GLN
1	B	278	ASN
1	B	385	ASN
1	C	53	GLN
1	C	211	GLN
1	C	304	GLN
1	C	362	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	E74	C	401	-	41,41,41	0.48	0	53,55,55	0.64	1 (1%)
2	E74	B	401	-	41,41,41	0.43	0	53,55,55	0.68	1 (1%)
2	E74	A	401	-	41,41,41	0.37	0	53,55,55	0.52	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
2	E74	C	401	-	-	3/36/36/36	0/3/4/4
2	E74	B	401	-	-	2/36/36/36	0/3/4/4
2	E74	A	401	-	-	2/36/36/36	0/3/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	401	E74	C47-C51-N54	-2.12	109.17	111.95
2	C	401	E74	C21-C18-C11	2.09	121.47	113.67

There are no chirality outliers.

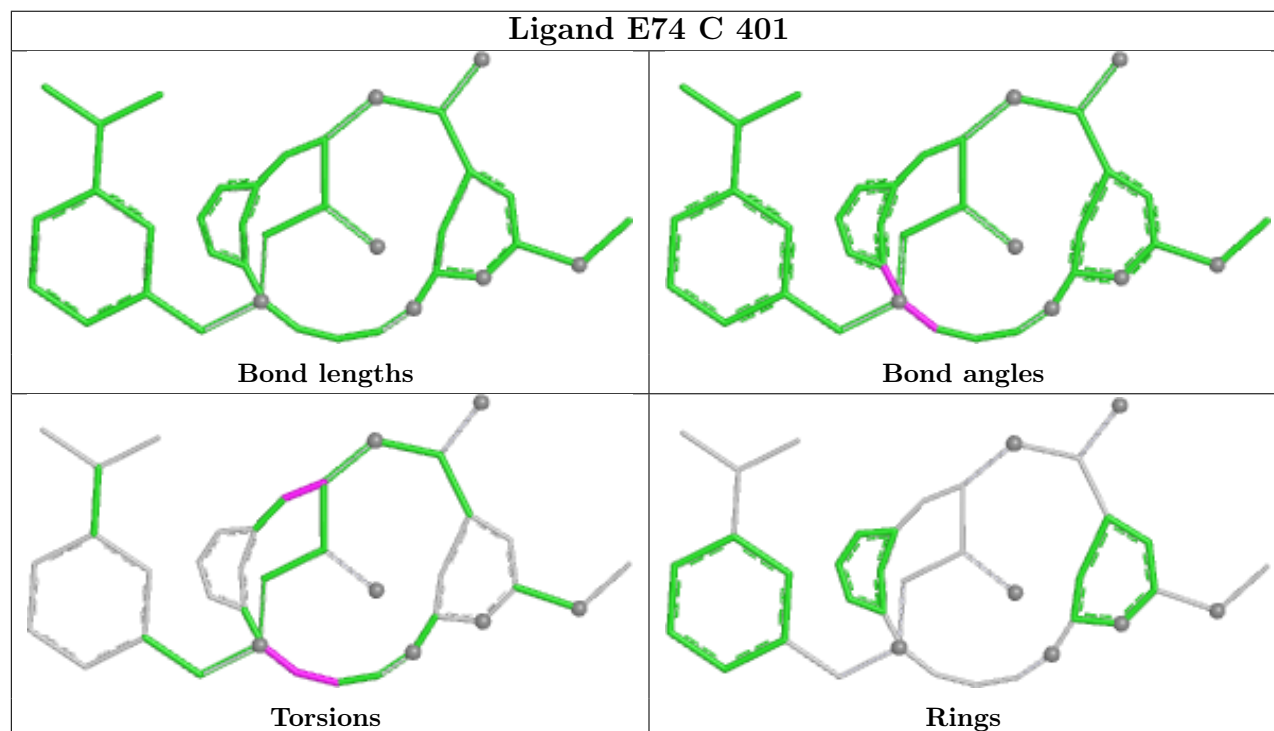
All (7) torsion outliers are listed below:

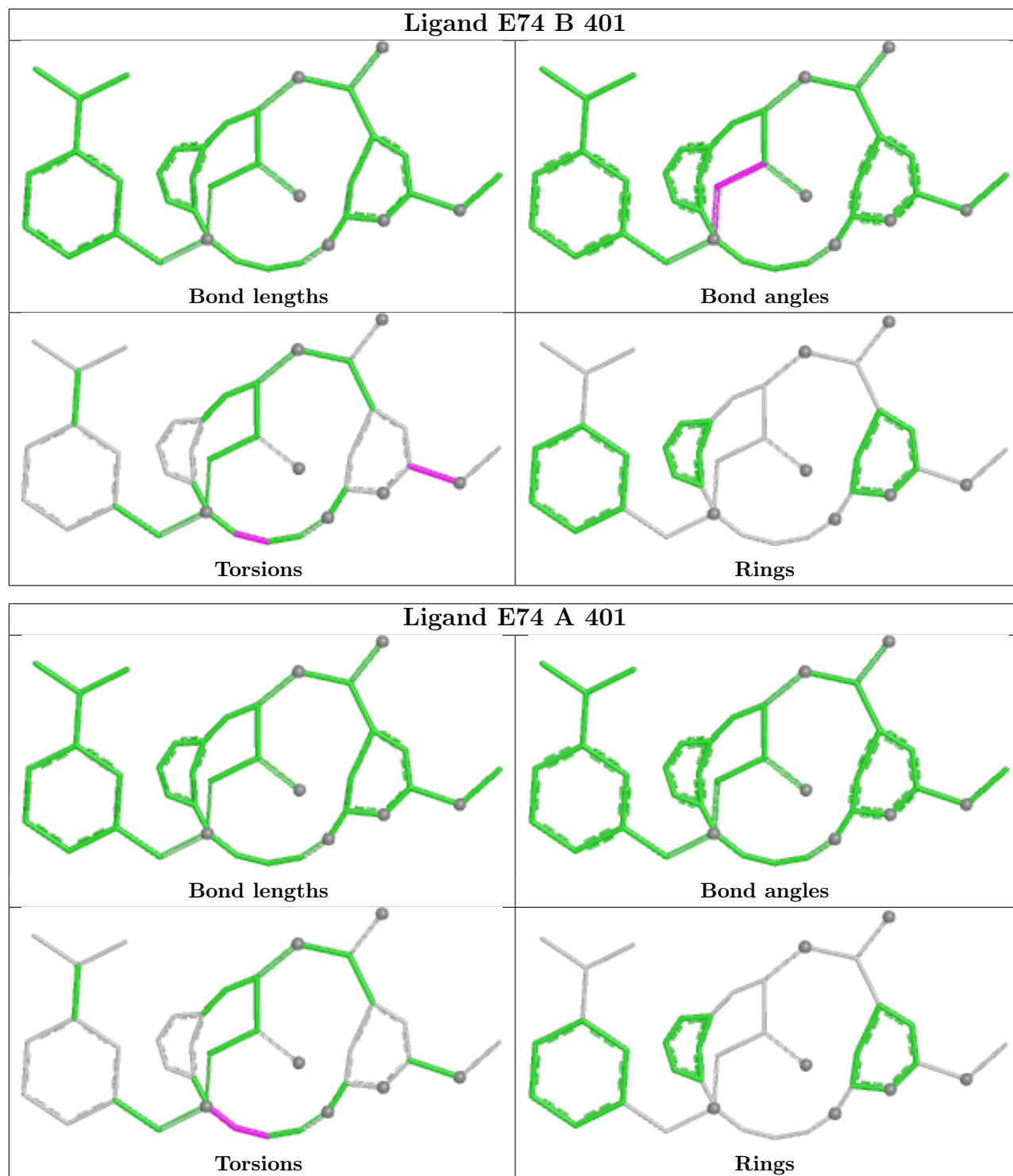
Mol	Chain	Res	Type	Atoms
2	C	401	E74	C11-C18-C21-C24
2	C	401	E74	C18-C21-C24-C27
2	A	401	E74	C11-C18-C21-C24
2	A	401	E74	C18-C21-C24-C27
2	B	401	E74	C18-C21-C24-C27
2	C	401	E74	N1-C3-C5-C8
2	B	401	E74	C35-C34-O42-C43

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 ⓘ

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	377/402 (93%)	0.15	23 (6%)	27 29	33, 47, 86, 176	0
1	B	377/402 (93%)	0.30	29 (7%)	19 21	30, 50, 109, 177	0
1	C	381/402 (94%)	0.23	24 (6%)	26 27	33, 47, 87, 158	0
All	All	1135/1206 (94%)	0.23	76 (6%)	24 25	30, 48, 96, 177	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	VAL	7.9
1	C	168	ALA	7.5
1	C	312	VAL	6.2
1	B	312	VAL	5.9
1	A	312	VAL	5.5
1	B	314	THR	5.2
1	C	362	HIS	5.2
1	A	365	PHE	5.0
1	A	362	HIS	5.0
1	B	365	PHE	4.7
1	C	314	THR	4.5
1	A	361	VAL	4.5
1	B	157	ALA	4.3
1	B	315	SER	3.9
1	C	313	ALA	3.8
1	A	254	THR	3.8
1	A	169	SER	3.8
1	A	317	ASP	3.7
1	C	315	SER	3.7
1	A	258	PRO	3.6
1	C	169	SER	3.6
1	B	380	GLU	3.6
1	B	258	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	365	PHE	3.5
1	C	159	PHE	3.4
1	C	160	PRO	3.3
1	B	-2	SER	3.2
1	A	73	GLN	3.2
1	B	362	HIS	3.2
1	B	267	LEU	3.2
1	B	254	THR	3.2
1	C	254	THR	3.1
1	B	73	GLN	3.1
1	B	317	ASP	3.1
1	C	311	ASP	3.1
1	B	313	ALA	3.1
1	C	361	VAL	3.0
1	B	169	SER	2.9
1	C	310	GLU	2.9
1	C	49	HIS	2.9
1	B	274	THR	2.9
1	A	313	ALA	2.8
1	A	314	THR	2.8
1	B	205	ARG	2.8
1	B	257	PHE	2.8
1	A	360	HIS	2.7
1	C	-2	SER	2.6
1	C	214	LYS	2.6
1	A	311	ASP	2.6
1	B	360	HIS	2.5
1	B	266	GLN	2.5
1	C	317	ASP	2.4
1	A	113	SER	2.4
1	A	315	SER	2.4
1	C	73	GLN	2.4
1	B	49	HIS	2.4
1	C	267	LEU	2.3
1	A	49	HIS	2.3
1	C	367	THR	2.3
1	A	359	CYS	2.3
1	B	340	GLY	2.3
1	C	359	CYS	2.3
1	B	272	ALA	2.3
1	C	158	GLY	2.3
1	C	258	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	273	GLY	2.2
1	B	268	VAL	2.2
1	B	263	LEU	2.2
1	B	113	SER	2.2
1	A	316	GLN	2.1
1	A	-2	SER	2.1
1	A	271	GLN	2.1
1	B	217	CYS	2.1
1	A	55	GLN	2.0
1	A	20	VAL	2.0
1	A	170	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

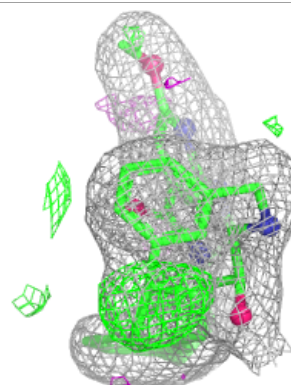
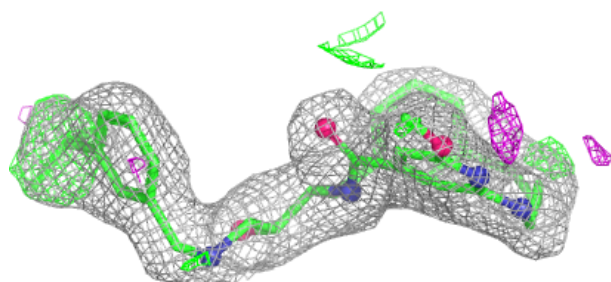
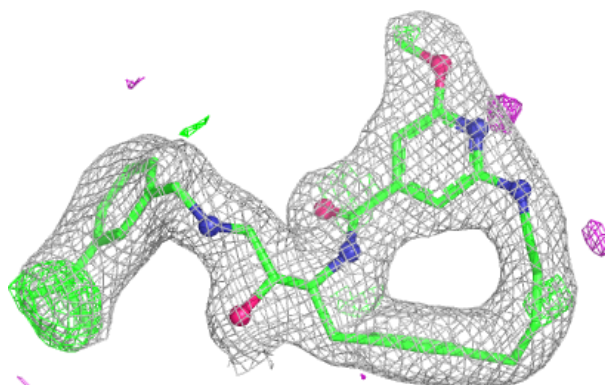
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	E74	B	401	38/38	0.94	0.10	34,41,52,53	3
2	E74	A	401	38/38	0.96	0.09	33,41,50,58	3
2	E74	C	401	38/38	0.97	0.07	35,42,47,56	1

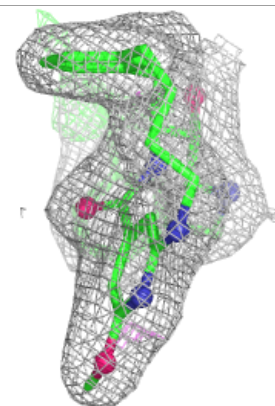
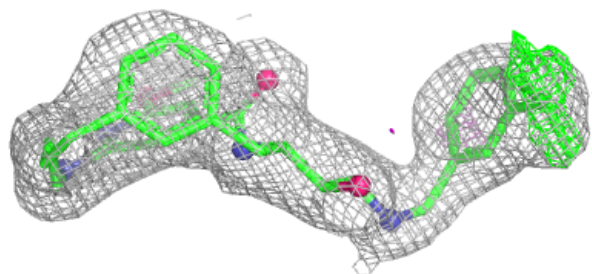
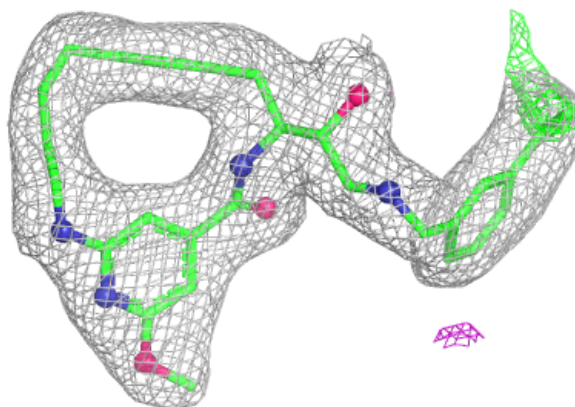
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around E74 B 401:

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

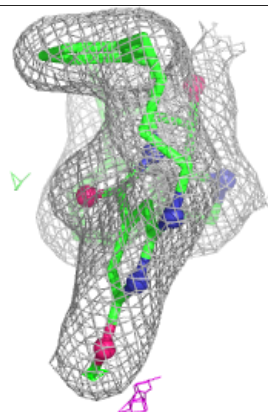
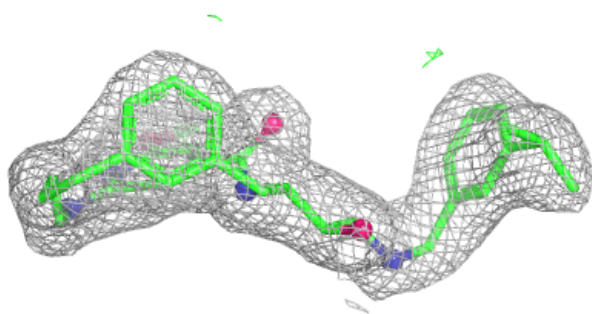
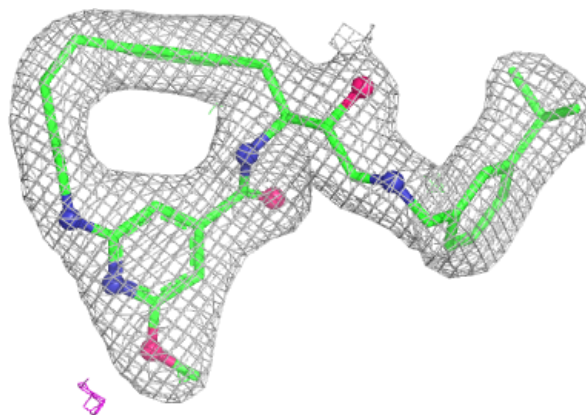
**Electron density around E74 A 401:**

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



Electron density around E74 C 401:

$2mF_o-DF_c$ (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.