



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:55 AM UTC

PDB ID : 4R8Y / pdb_00004r8y
Title : BACE-1 in complex with (R)-4-(2-cyclohexylethyl)-4-(((R)-1-(2-cyclopentylacetyl)pyrrolidin-3-yl)methyl)-1-methyl-5-oxoimidazolidin-2-iminium
Authors : Orth, P.; Caldwell, J.P.; Strickland, C.
Deposited on : 2014-09-03
Resolution : 1.90 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 ⓘ 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

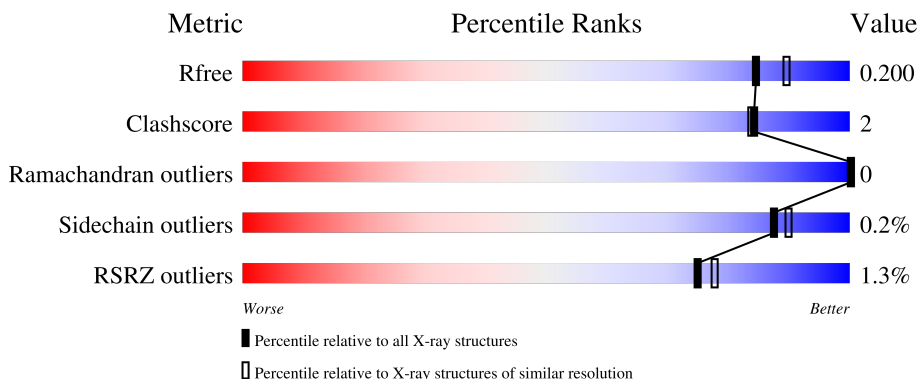
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	414	% 86% 7% 7%
1	B	414	% 90% • 7%

2 Entry composition [i](#)

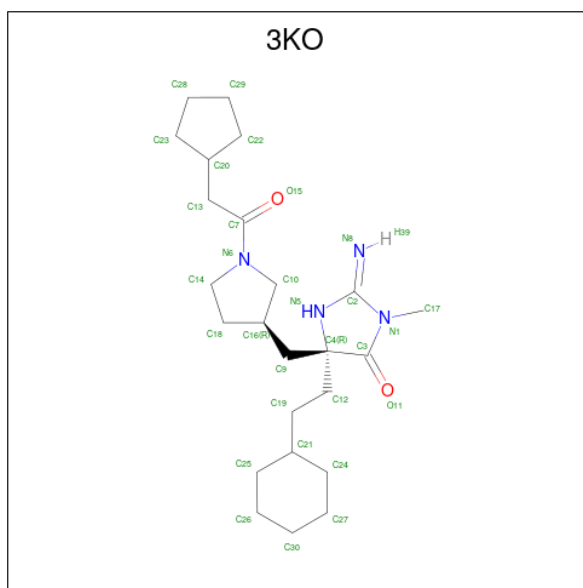
There are 4 unique types of molecules in this entry. The entry contains 6964 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

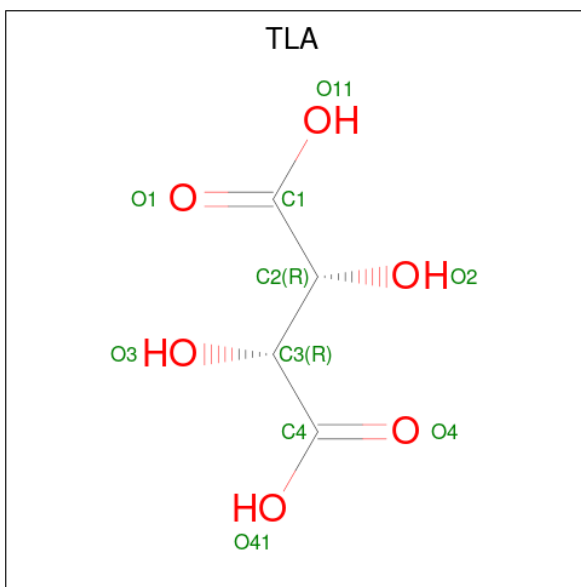
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3015	1932	498	571	14			
1	B	387	Total	C	N	O	S	0	0	0
			3024	1936	503	571	14			

- Molecule 2 is (2E,5R)-5-(2-cyclohexylethyl)-5-[(3R)-1-(cyclopentylacetyl)pyrrolidin-3-yl]methyl}-2-imino-3-methylimidazolidin-4-one (CCD ID: 3KO) (formula: C₂₄H₄₀N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	24	4	2		
2	B	1	Total	C	N	O	0	0
			30	24	4	2		

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	415	Total	O	0	0
			415	415		
4	B	440	Total	O	0	0
			440	440		

- Molecule 1: Beta-secretase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.40Å 89.43Å 131.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 1.90 19.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.90-1.90) 95.5 (19.90-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 1.90Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.11.4	Depositor
R, R_{free}	0.174 , 0.205 0.170 , 0.200	Depositor DCC
R_{free} test set	3864 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6964	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5508e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 3KO, TLA

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	0.79	0/3091	0.99	8/4205 (0.2%)
1	B	0.81	0/3101	1.01	6/4217 (0.1%)
All	All	0.80	0/6192	1.00	14/8422 (0.2%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	TYR	N-CA-C	-6.09	101.95	110.35
1	B	294	ASN	N-CA-C	5.94	118.19	110.53
1	A	294	ASN	N-CA-C	5.92	118.17	110.53
1	A	259	TYR	N-CA-C	-5.91	102.20	110.35
1	A	295	LEU	N-CA-C	-5.83	99.64	108.67

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	3015	0	2900	17	0
1	B	3024	0	2909	10	0
2	A	30	0	39	1	0
2	B	30	0	39	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	4	0	0
4	A	415	0	0	1	0
4	B	440	0	0	1	0
All	All	6964	0	5891	27	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.

The worst 5 of 27 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:361:ILE:HD13	1:A:398:ILE:HD12	1.83	0.60
1:B:171:ILE:HD11	2:B:502:3KO:H37	1.84	0.59
1:B:361:ILE:HD13	1:B:398:ILE:HD12	1.85	0.58
1:A:125:ARG:HD3	4:A:863:HOH:O	2.05	0.56
1:A:63:MET:HG2	1:A:151:GLY:HA2	1.90	0.53

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	383/414 (92%)	376 (98%)	7 (2%)	0	100	100
1	B	383/414 (92%)	376 (98%)	7 (2%)	0	100	100
All	All	766/828 (92%)	752 (98%)	14 (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	323/355 (91%)	322 (100%)	1 (0%)	86	88
1	B	324/355 (91%)	324 (100%)	0	100	100
All	All	647/710 (91%)	646 (100%)	1 (0%)	87	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	294	ASN
1	B	446	ASN
1	A	294	ASN
1	A	446	ASN
1	B	172	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	3KO	B	502	-	31,33,33	0.69	1 (3%)	33,47,47	1.14	2 (6%)
2	3KO	A	501	-	31,33,33	0.74	1 (3%)	33,47,47	1.21	2 (6%)
3	TLA	B	501	-	9,9,9	2.61	5 (55%)	12,12,12	1.63	3 (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	3KO	B	502	-	-	4/19/62/62	0/4/4/4
2	3KO	A	501	-	-	4/19/62/62	0/4/4/4
3	TLA	B	501	-	-	0/12/12/12	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	TLA	O1-C1	4.70	1.36	1.22
3	B	501	TLA	O4-C4	3.29	1.31	1.22
3	B	501	TLA	O41-C4	-3.22	1.20	1.30
3	B	501	TLA	O2-C2	2.91	1.47	1.42
3	B	501	TLA	O11-C1	-2.45	1.22	1.30

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	3KO	O11-C3-C4	-3.03	124.08	126.75
3	B	501	TLA	O41-C4-C3	2.85	121.23	113.31
3	B	501	TLA	O41-C4-O4	-2.80	117.72	124.08
2	A	501	3KO	C4-N5-C2	-2.76	111.06	113.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	3KO	C19-C21-C25	-2.53	105.69	112.05

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

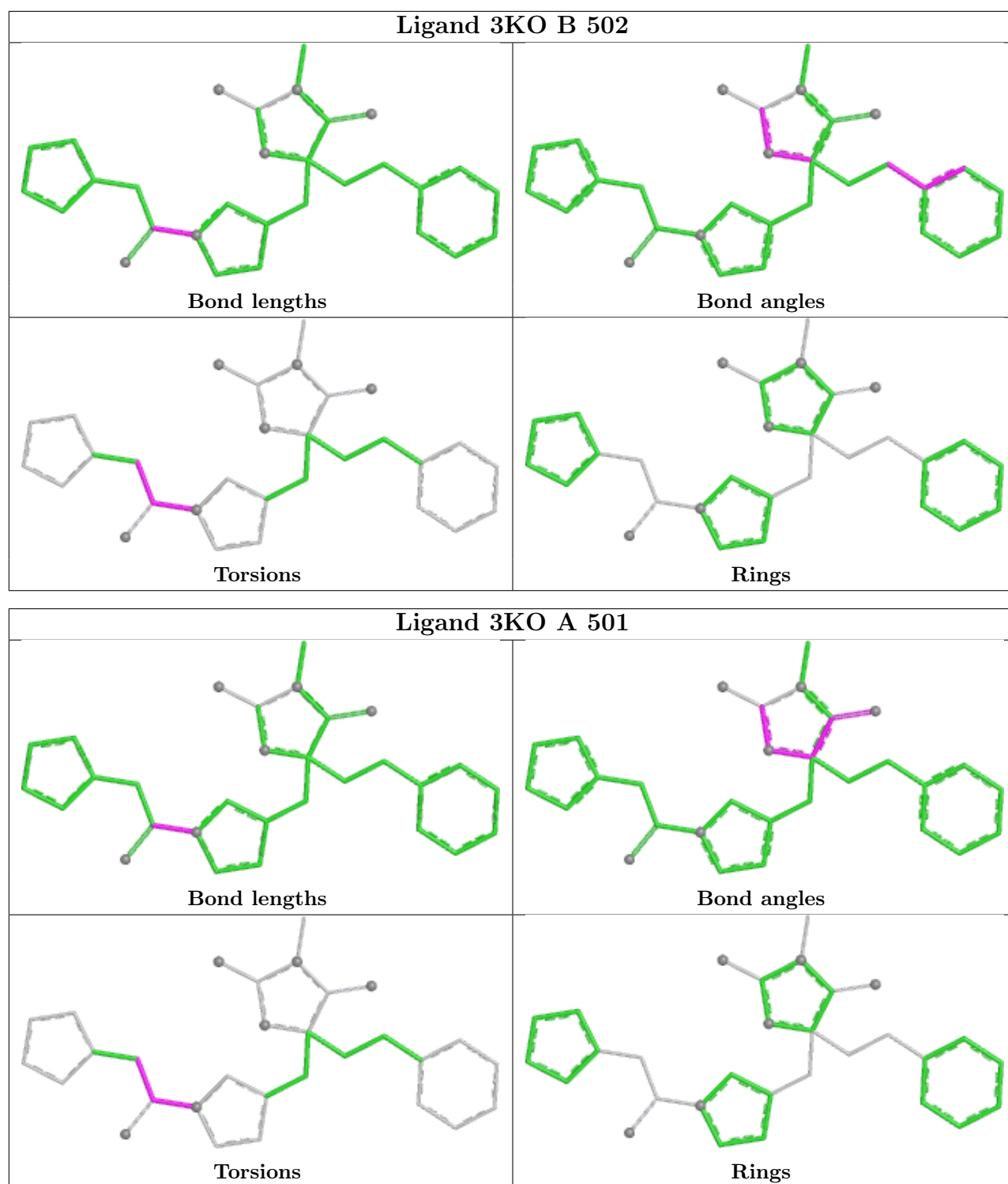
Mol	Chain	Res	Type	Atoms
2	A	501	3KO	C13-C7-N6-C10
2	A	501	3KO	O15-C7-N6-C10
2	B	502	3KO	C13-C7-N6-C14
2	B	502	3KO	O15-C7-N6-C14
2	A	501	3KO	C20-C13-C7-O15

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	3KO	2	0
2	A	501	3KO	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 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 ⓘ

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	387/414 (93%)	-0.36	5 (1%) 75 78	12, 19, 36, 85	0
1	B	387/414 (93%)	-0.37	5 (1%) 75 78	12, 19, 35, 57	0
All	All	774/828 (93%)	-0.37	10 (1%) 75 78	12, 19, 36, 85	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	ILE	6.8
1	B	372	ASP	2.9
1	B	133	THR	2.8
1	B	206	HIS	2.6
1	A	129	TYR	2.2

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](#)

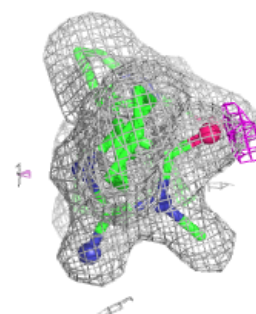
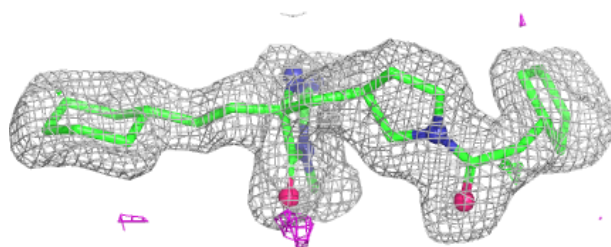
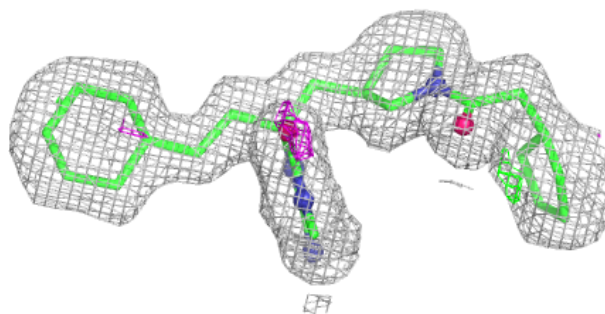
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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
3	TLA	B	501	10/10	0.90	0.08	38,42,44,45	0
2	3KO	A	501	30/30	0.94	0.07	14,22,28,31	0
2	3KO	B	502	30/30	0.96	0.06	13,18,25,26	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.

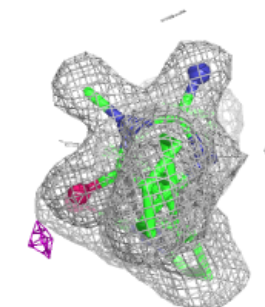
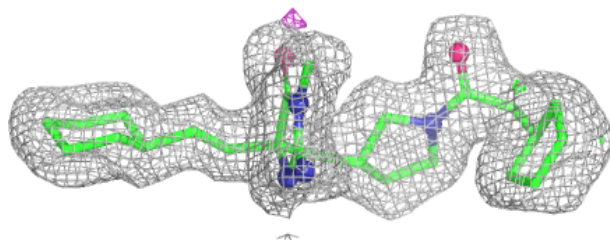
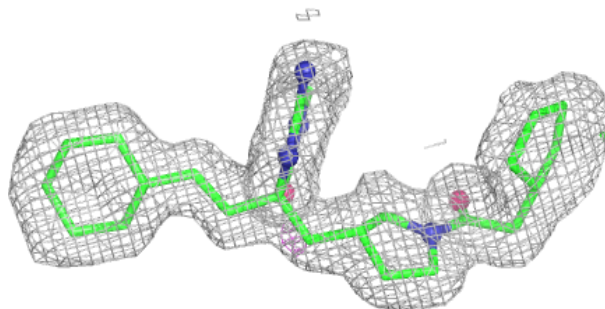
Electron density around 3KO A 501:

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 3KO B 502:

$2mF_o-DF_c$ (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.