



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:12 PM UTC

PDB ID : 3MSK / pdb_00003msk
Title : Fragment Based Discovery and Optimisation of BACE-1 Inhibitors
Authors : Smith, M.A.; Madden, J.M.; Barker, J.; Godemann, R.; Kraemer, J.; Hallett, D.
Deposited on : 2010-04-29
Resolution : 2.00 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

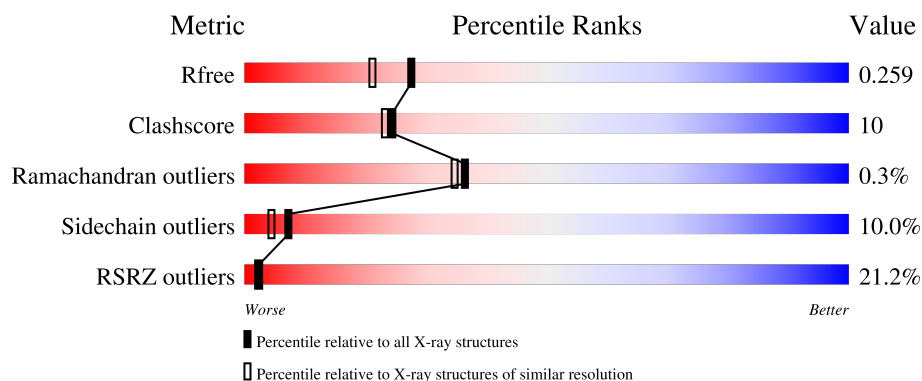
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	408	20% 69% 18% • • 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3275 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
			Total	C	N	O	S			
1	A	378	2984	1911	495	564	14	29	3	1

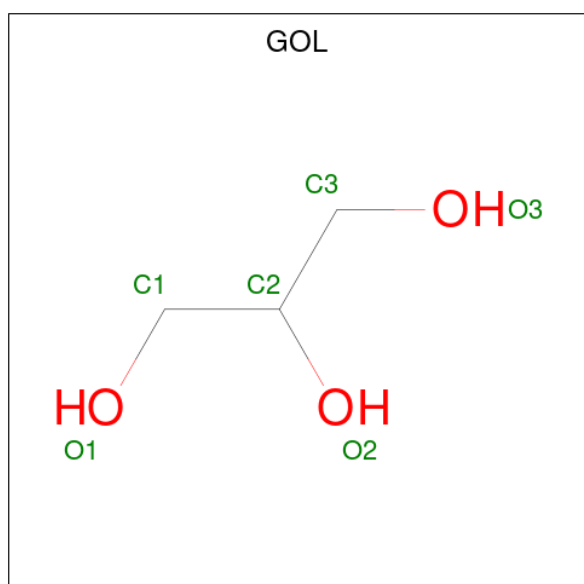
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

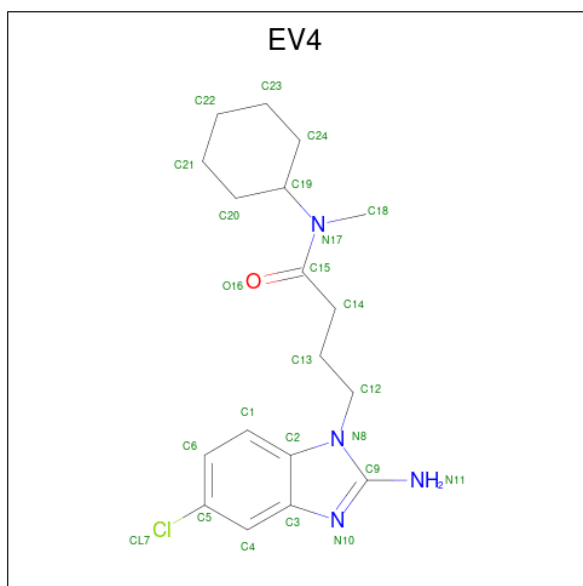
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total I 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 4-(2-amino-5-chloro-1H-benzimidazol-1-yl)-N-cyclohexyl-N-methylbutanamide (CCD ID: EV4) (formula: $C_{18}H_{25}ClN_4O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			24	18	1	4	1		

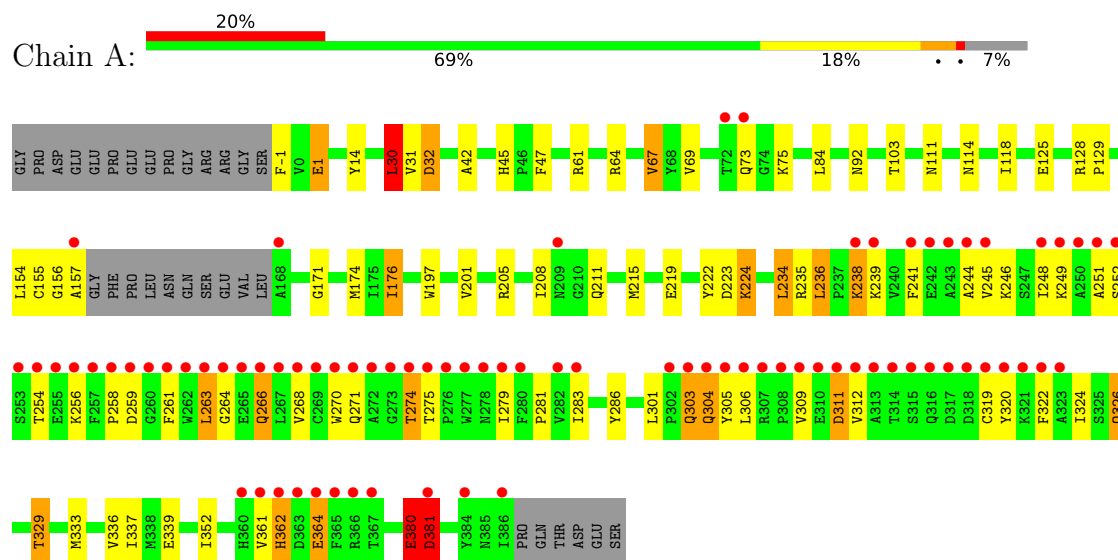
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	260	Total	O	0	0
			260	260		

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: Beta-secretase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.51Å 102.51Å 170.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.09 – 2.00 49.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.09-2.00) 100.0 (49.09-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.223 , 0.264 0.222 , 0.259	Depositor DCC
R_{free} test set	1825 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3275	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: EV4, IOD, GOL

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	1.52	13/3064 (0.4%)	1.21	10/4166 (0.2%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	GLU	C-N	-32.18	0.90	1.34
1	A	381	ASP	C-N	-22.41	1.03	1.33
1	A	238	LYS	CD-CE	-7.41	1.30	1.52
1	A	69	VAL	CA-CB	6.32	1.62	1.54
1	A	61	ARG	C-O	5.47	1.30	1.24
1	A	309	VAL	CA-CB	5.44	1.59	1.53
1	A	32	ASP	C-O	5.40	1.30	1.23
1	A	329	THR	CA-CB	5.40	1.61	1.53
1	A	30	LEU	CA-C	5.37	1.59	1.52
1	A	45	HIS	CA-C	5.33	1.58	1.53
1	A	266	GLN	CB-CG	-5.24	1.36	1.52
1	A	42	ALA	N-CA	5.13	1.52	1.46
1	A	84	LEU	C-O	5.03	1.30	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	GLU	O-C-N	9.28	133.69	122.27
1	A	266	GLN	CB-CG-CD	7.73	125.75	112.60
1	A	311	ASP	N-CA-C	6.84	119.88	109.62
1	A	381	ASP	O-C-N	-6.55	114.56	122.22
1	A	364	GLU	N-CA-C	6.03	117.53	111.07
1	A	380	GLU	CA-C-N	-5.81	111.91	120.28
1	A	380	GLU	C-N-CA	-5.81	111.91	120.28
1	A	211	GLN	N-CA-C	5.62	117.57	108.41
1	A	339	GLU	N-CA-C	5.52	118.06	111.71
1	A	236	LEU	N-CA-C	5.08	117.87	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	TRP	Peptide
1	A	381	ASP	Mainchain

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	2984	0	2899	54	1
2	A	1	0	0	0	0
3	A	6	0	7	0	0
4	A	24	0	25	5	0
5	A	260	0	0	10	0
All	All	3275	0	2931	58	1

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 10.

All (58) 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:30:LEU:C	1:A:30:LEU:HD23	1.96	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:396:EV4:H24	4:A:396:EV4:C14	2.07	0.84
4:A:396:EV4:H24	4:A:396:EV4:H14A	1.64	0.77
1:A:301:LEU:HB2	1:A:303:GLN:HG2	1.72	0.70
1:A:30:LEU:HD23	1:A:31:VAL:N	2.05	0.70
1:A:362:HIS:NE2	5:A:613:HOH:O	2.28	0.67
1:A:281:PRO:HD2	1:A:305:TYR:OH	1.95	0.65
1:A:224:LYS:HZ1	1:A:329:THR:HB	1.63	0.63
1:A:215:MET:HE2	1:A:219:GLU:HG3	1.80	0.62
1:A:244:ALA:O	1:A:248:ILE:HG13	1.99	0.62
1:A:67:VAL:CG1	1:A:129:PRO:HD3	2.31	0.61
1:A:224:LYS:NZ	1:A:329:THR:O	2.32	0.60
1:A:333:MET:HE2	1:A:337:ILE:HG21	1.82	0.60
1:A:114:ASN:ND2	5:A:535:HOH:O	2.33	0.59
1:A:30:LEU:C	1:A:30:LEU:CD2	2.74	0.59
1:A:241:PHE:CD2	1:A:326:GLN:HG2	2.38	0.59
1:A:268:VAL:O	1:A:319:CYS:HA	2.05	0.57
1:A:224:LYS:NZ	1:A:329:THR:HB	2.19	0.57
1:A:245:VAL:O	1:A:249:LYS:N	2.31	0.57
1:A:156:GLY:O	1:A:157:ALA:HB3	2.03	0.56
1:A:251:ALA:HB3	5:A:592:HOH:O	2.03	0.56
4:A:396:EV4:C14	4:A:396:EV4:C24	2.79	0.56
1:A:1:GLU:HB3	5:A:446:HOH:O	2.05	0.55
1:A:215:MET:CE	1:A:219:GLU:HG3	2.36	0.55
1:A:261:PHE:CE1	1:A:322:PHE:HB2	2.42	0.54
1:A:236:LEU:O	1:A:326:GLN:HA	2.08	0.53
1:A:270:TRP:HZ3	1:A:320:TYR:CD1	2.27	0.53
1:A:301:LEU:CB	1:A:303:GLN:HG2	2.39	0.52
1:A:252:SER:HA	1:A:279:ILE:HG22	1.89	0.52
1:A:245:VAL:HA	1:A:248:ILE:HB	1.92	0.52
1:A:235:ARG:NE	5:A:506:HOH:O	2.44	0.51
1:A:205:ARG:HB3	1:A:286:TYR:HB2	1.94	0.49
1:A:270:TRP:HZ3	1:A:320:TYR:HD1	1.60	0.48
1:A:155:CYS:HB2	1:A:171:GLY:O	2.14	0.48
1:A:333:MET:CE	1:A:337:ILE:HG21	2.44	0.48
1:A:245:VAL:O	1:A:246:LYS:C	2.56	0.47
1:A:67:VAL:HG13	1:A:129:PRO:HD3	1.97	0.46
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.96	0.46
1:A:268:VAL:HG13	1:A:270:TRP:CH2	2.51	0.46
1:A:234:LEU:O	1:A:324:ILE:HA	2.16	0.46
1:A:-1:PHE:N	5:A:617:HOH:O	2.48	0.45
1:A:258:PRO:O	1:A:261:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:396:EV4:H20A	4:A:396:EV4:H18	1.57	0.45
1:A:264:GLY:HA2	5:A:553:HOH:O	2.16	0.45
1:A:129:PRO:HB3	5:A:641:HOH:O	2.15	0.45
1:A:215:MET:HE2	1:A:215:MET:HB3	1.84	0.45
1:A:32:ASP:OD2	4:A:396:EV4:N10	2.51	0.44
1:A:222:TYR:HA	1:A:223:ASP:HA	1.39	0.44
1:A:281:PRO:HD3	5:A:592:HOH:O	2.18	0.44
1:A:380:GLU:O	1:A:381:ASP:C	2.54	0.44
1:A:201:VAL:CG1	1:A:352:ILE:HD12	2.49	0.43
1:A:304:GLN:O	1:A:336:VAL:HG22	2.19	0.42
1:A:47:PHE:CE2	1:A:111:ASN:HB2	2.54	0.42
1:A:103:THR:HB	5:A:590:HOH:O	2.19	0.42
1:A:259:ASP:O	1:A:263:LEU:HD22	2.20	0.41
1:A:32:ASP:OD2	1:A:118:ILE:HD11	2.21	0.41
1:A:238:LYS:HB2	1:A:238:LYS:HE2	1.90	0.40
1:A:14:TYR:CZ	1:A:154:LEU:HB3	2.56	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:NZ	1:A:238:LYS:NZ[12_545]	2.06	0.14

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	377/408 (92%)	363 (96%)	13 (3%)	1 (0%)	36	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	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	Percentiles
1	A	324/348 (93%)	292 (90%)	32 (10%)	7 4

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	30	LEU
1	A	64	ARG
1	A	67	VAL
1	A	73	GLN
1	A	75	LYS
1	A	92	ASN
1	A	125	GLU
1	A	128	ARG
1	A	176	ILE
1	A	208	ILE
1	A	224	LYS
1	A	234	LEU
1	A	239	LYS
1	A	254	THR
1	A	256	LYS
1	A	263	LEU
1	A	266	GLN
1	A	271	GLN
1	A	274	THR
1	A	275	THR
1	A	283	ILE
1	A	303	GLN
1	A	304	GLN
1	A	306	LEU
1	A	311	ASP

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Mol	Chain	Res	Type
1	A	312	VAL
1	A	326	GLN
1	A	361	VAL
1	A	362	HIS
1	A	364	GLU
1	A	380	GLU

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

Mol	Chain	Res	Type
1	A	12	GLN
1	A	89	HIS
1	A	114	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 [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	GOL	A	394	-	5,5,5	1.26	1 (20%)	5,5,5	1.08	0
4	EV4	A	396	-	26,26,26	1.90	3 (11%)	33,36,36	2.12	7 (21%)

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	GOL	A	394	-	-	3/4/4/4	-
4	EV4	A	396	-	-	5/14/22/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	396	EV4	C2-C3	6.90	1.51	1.40
4	A	396	EV4	C9-N10	4.05	1.37	1.32
3	A	394	GOL	O2-C2	-2.63	1.35	1.43
4	A	396	EV4	C3-N10	-2.53	1.34	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	396	EV4	N11-C9-N10	-7.38	118.38	124.78
4	A	396	EV4	C23-C24-C19	-4.31	102.60	110.81
4	A	396	EV4	C3-C2-N8	3.37	108.22	105.55
4	A	396	EV4	C12-N8-C9	2.96	132.48	125.23
4	A	396	EV4	C1-C2-C3	-2.82	118.98	122.23
4	A	396	EV4	C21-C20-C19	-2.53	105.99	110.81
4	A	396	EV4	C2-C3-N10	-2.26	107.31	110.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	396	EV4	C20-C19-N17-C15
4	A	396	EV4	C24-C19-N17-C15
4	A	396	EV4	C20-C19-N17-C18
4	A	396	EV4	C24-C19-N17-C18
3	A	394	GOL	O1-C1-C2-C3

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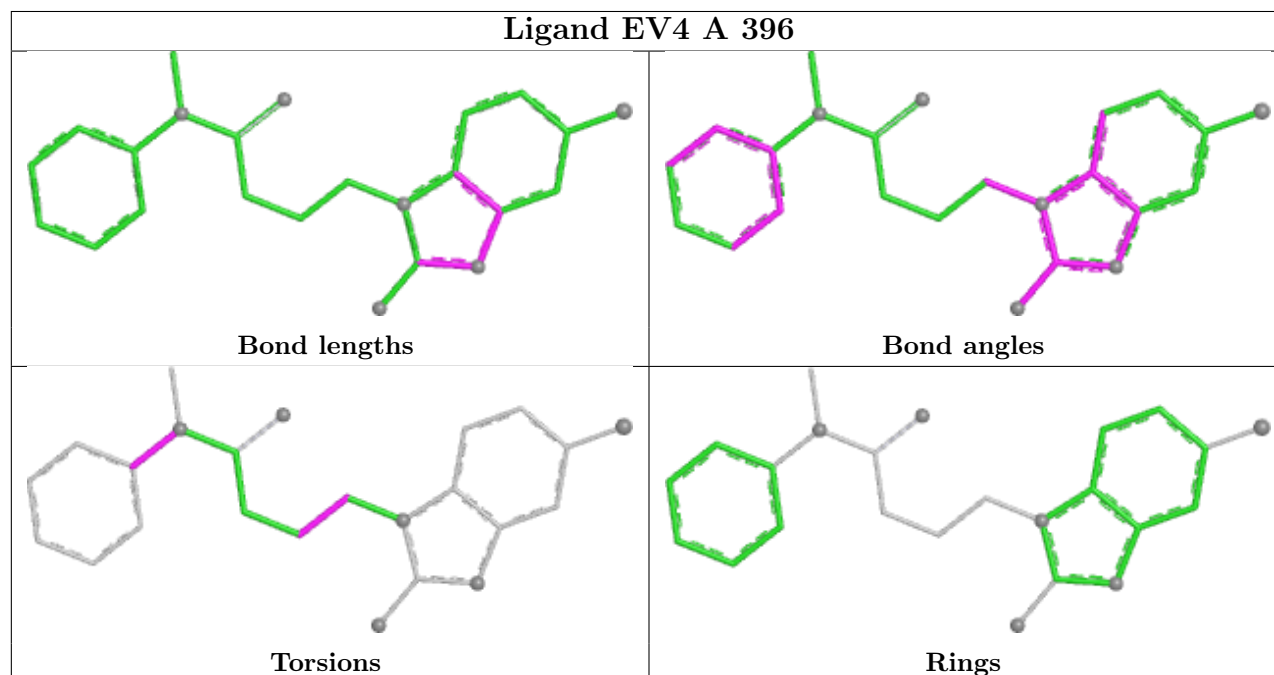
Mol	Chain	Res	Type	Atoms
4	A	396	EV4	N8-C12-C13-C14
3	A	394	GOL	O1-C1-C2-O2
3	A	394	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	396	EV4	5	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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	381:ASP	C	382:CYS	N	1.03
1	A	380:GLU	C	381:ASP	N	0.90

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	378/408 (92%)	0.73	80 (21%) 2 2	9, 30, 96, 125	13 (3%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	VAL	7.1
1	A	314	THR	7.0
1	A	272	ALA	6.7
1	A	313	ALA	6.6
1	A	270	TRP	6.4
1	A	279	ILE	6.4
1	A	309	VAL	6.3
1	A	73	GLN	5.7
1	A	258	PRO	5.5
1	A	365	PHE	5.5
1	A	274	THR	5.2
1	A	260	GLY	5.1
1	A	271	GLN	4.9
1	A	267	LEU	4.8
1	A	306	LEU	4.8
1	A	250	ALA	4.7
1	A	277	TRP	4.7
1	A	319	CYS	4.6
1	A	254	THR	4.5
1	A	245	VAL	4.5
1	A	268	VAL	4.4
1	A	251	ALA	4.2
1	A	320	TYR	4.1
1	A	311	ASP	4.1
1	A	275	THR	4.0
1	A	252	SER	4.0
1	A	157	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	317	ASP	3.9
1	A	362	HIS	3.7
1	A	168	ALA	3.7
1	A	276	PRO	3.7
1	A	315	SER	3.7
1	A	318	ASP	3.6
1	A	273	GLY	3.6
1	A	316	GLN	3.5
1	A	384	TYR	3.5
1	A	244	ALA	3.4
1	A	308	PRO	3.4
1	A	280	PHE	3.4
1	A	269	CYS	3.4
1	A	367	THR	3.3
1	A	323	ALA	3.2
1	A	361	VAL	3.2
1	A	310	GLU	3.2
1	A	249	LYS	3.2
1	A	257	PHE	3.1
1	A	364	GLU	3.1
1	A	261	PHE	3.1
1	A	259	ASP	3.1
1	A	302	PRO	3.0
1	A	253	SER	3.0
1	A	305	TYR	3.0
1	A	386	ILE	2.9
1	A	303	GLN	2.9
1	A	307	ARG	2.9
1	A	278	ASN	2.9
1	A	321	LYS	2.9
1	A	263	LEU	2.8
1	A	238	LYS	2.7
1	A	283	ILE	2.6
1	A	266	GLN	2.6
1	A	243	ALA	2.6
1	A	239	LYS	2.6
1	A	255	GLU	2.5
1	A	304	GLN	2.5
1	A	360	HIS	2.5
1	A	322	PHE	2.5
1	A	256	LYS	2.5
1	A	248	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	262	TRP	2.4
1	A	241	PHE	2.4
1	A	282	VAL	2.4
1	A	264	GLY	2.3
1	A	72	THR	2.2
1	A	366	ARG	2.2
1	A	209	ASN	2.1
1	A	381	ASP	2.1
1	A	265	GLU	2.0
1	A	242	GLU	2.0
1	A	363	ASP	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](#)

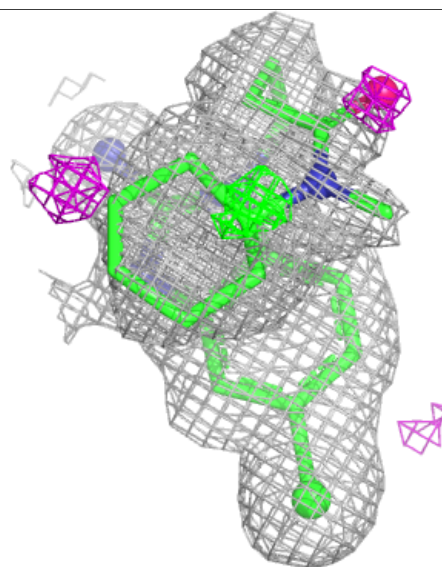
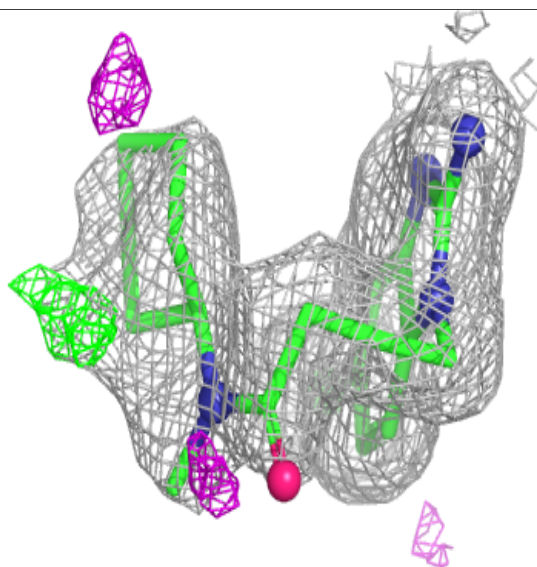
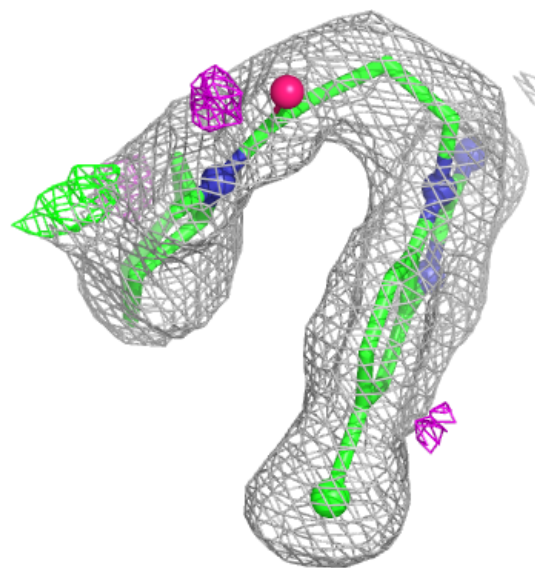
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	EV4	A	396	24/24	0.91	0.15	23,42,58,61	0
3	GOL	A	394	6/6	0.94	0.23	30,41,50,60	0
2	IOD	A	393	1/1	1.00	0.04	38,38,38,38	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 EV4 A 396:

$2mF_o-DF_c$ (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.