



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:12 PM UTC

PDB ID : 2QU2 / pdb_00002qu2
Title : BACE1 with Compound 1
Authors : Chopra, R.
Deposited on : 2007-08-03
Resolution : 2.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

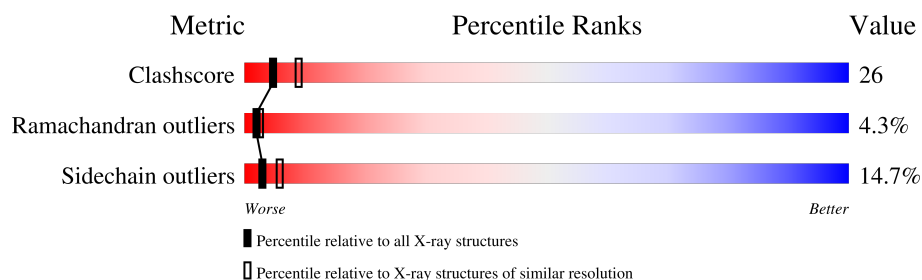
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	415	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3034 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.

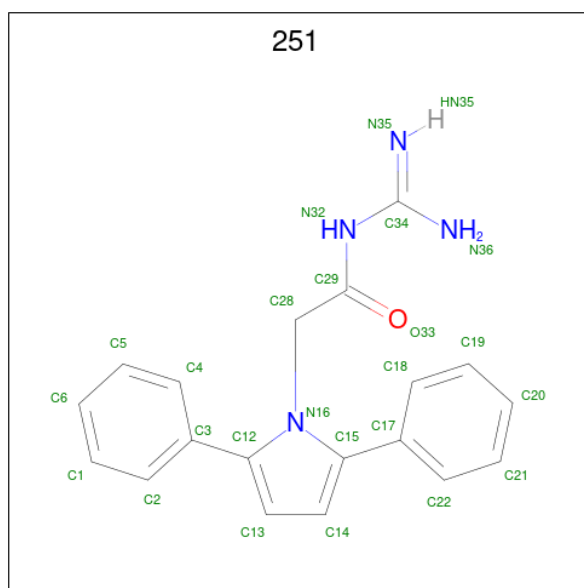
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	2854	1834	475	532	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	HIS	-	expression tag	UNP P56817
A	457	HIS	-	expression tag	UNP P56817
A	458	HIS	-	expression tag	UNP P56817
A	459	HIS	-	expression tag	UNP P56817
A	460	HIS	-	expression tag	UNP P56817
A	461	HIS	-	expression tag	UNP P56817

- Molecule 2 is N-[amino(imino)methyl]-2-(2,5-diphenyl-1H-pyrrol-1-yl)acetamide (CCD ID: 251) (formula: C₁₉H₁₈N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	19	4	1		

- Molecule 3 is water.

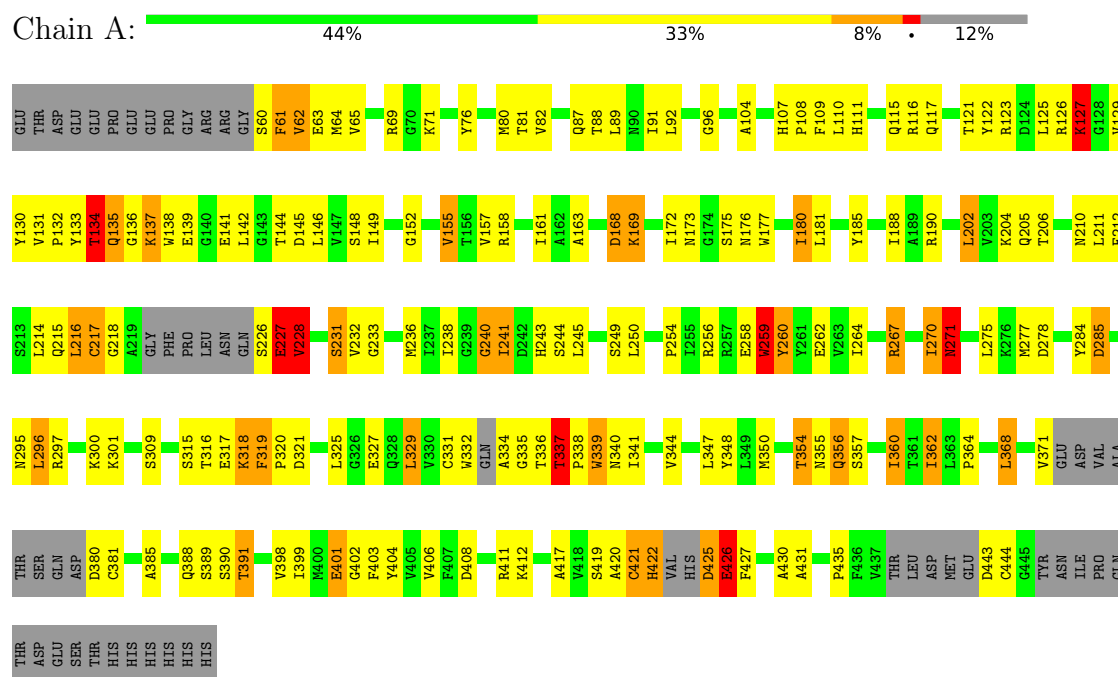
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	156	Total	O	0	0
			156	156		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: Beta-secretase 1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.92Å 104.84Å 50.48Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.60	Depositor
% Data completeness (in resolution range)	96.7 (19.95-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3034	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
251

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	0.60	4/2923 (0.1%)	1.21	41/3966 (1.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	ASN	C-O	8.13	1.34	1.24
1	A	271	ASN	CB-CG	7.81	1.71	1.52
1	A	271	ASN	CA-C	5.39	1.59	1.52
1	A	270	ILE	CA-C	-5.10	1.48	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	ALA	N-CA-C	-10.88	99.50	111.36
1	A	226	SER	CA-C-N	9.57	139.82	121.54
1	A	226	SER	C-N-CA	9.57	139.82	121.54
1	A	444	CYS	N-CA-C	8.68	123.99	113.23
1	A	337	THR	CA-C-N	8.52	130.48	119.84
1	A	337	THR	C-N-CA	8.52	130.48	119.84
1	A	141	GLU	N-CA-C	-7.70	96.39	109.24
1	A	271	ASN	N-CA-C	7.54	126.86	110.80
1	A	217	CYS	N-CA-C	7.45	122.50	113.41
1	A	227	GLU	CA-CB-CG	-7.42	99.26	114.10
1	A	430	ALA	N-CA-C	-7.16	100.40	110.50
1	A	260	TYR	N-CA-C	-7.06	99.41	110.36
1	A	271	ASN	CA-C-O	6.94	130.44	120.51
1	A	426	GLU	N-CA-C	6.89	120.26	110.68
1	A	278	ASP	N-CA-C	-6.74	99.85	109.96
1	A	61	PHE	N-CA-C	-6.69	96.56	110.80
1	A	270	ILE	N-CA-C	-6.67	97.12	106.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	THR	N-CA-C	-6.37	105.44	113.72
1	A	227	GLU	N-CA-CB	6.31	121.15	110.49
1	A	340	ASN	N-CA-C	6.27	120.53	113.01
1	A	360	ILE	N-CA-C	-6.21	99.41	108.11
1	A	71	LYS	N-CA-C	-6.20	99.60	109.59
1	A	421	CYS	N-CA-C	-6.20	101.76	110.50
1	A	270	ILE	CA-C-N	6.13	133.25	121.54
1	A	270	ILE	C-N-CA	6.13	133.25	121.54
1	A	185	TYR	N-CA-C	5.96	118.39	110.53
1	A	296	LEU	N-CA-C	-5.81	99.06	108.41
1	A	270	ILE	O-C-N	5.70	130.47	122.20
1	A	188	ILE	N-CA-C	5.69	117.64	112.29
1	A	354	THR	N-CA-C	5.62	122.76	110.80
1	A	125	LEU	N-CA-C	-5.61	107.07	114.31
1	A	295	ASN	N-CA-C	5.59	117.91	110.53
1	A	111	HIS	N-CA-C	-5.58	105.83	113.30
1	A	271	ASN	CA-C-N	5.37	131.74	123.31
1	A	271	ASN	C-N-CA	5.37	131.74	123.31
1	A	381	CYS	N-CA-C	5.36	118.81	110.17
1	A	243	HIS	N-CA-C	5.35	118.91	112.38
1	A	127	LYS	N-CA-C	-5.34	99.42	110.80
1	A	91	ILE	N-CA-C	5.30	115.49	107.75
1	A	259	TRP	N-CA-C	-5.21	99.71	110.80
1	A	240	GLY	N-CA-C	5.16	118.07	110.80

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	2854	0	2777	146	0
2	A	24	0	18	3	0
3	A	156	0	0	6	0
All	All	3034	0	2795	146	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 26.

All (146) 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:144:THR:HG23	1:A:158:ARG:NH1	1.70	1.07
1:A:127:LYS:HG2	1:A:142:LEU:HD12	1.46	0.97
1:A:421:CYS:O	1:A:422:HIS:HB3	1.69	0.92
1:A:123:ARG:HB2	1:A:144:THR:HG22	1.57	0.87
1:A:61:PHE:H	1:A:64:MET:HE3	1.39	0.87
1:A:64:MET:HG2	1:A:152:GLY:HA2	1.58	0.85
1:A:321:ASP:O	1:A:325:LEU:HD23	1.78	0.83
1:A:315:SER:C	1:A:317:GLU:H	1.85	0.83
1:A:227:GLU:O	1:A:228:VAL:O	1.96	0.82
1:A:332:TRP:O	1:A:334:ALA:N	2.12	0.81
1:A:144:THR:HG23	1:A:158:ARG:HH11	1.42	0.81
1:A:134:THR:O	1:A:135:GLN:HB2	1.80	0.81
1:A:227:GLU:C	1:A:228:VAL:CG2	2.53	0.81
1:A:136:GLY:HA2	1:A:168:ASP:HB3	1.64	0.80
1:A:136:GLY:HA3	1:A:168:ASP:O	1.87	0.75
1:A:107:HIS:CD2	1:A:109:PHE:H	2.05	0.73
1:A:318:LYS:HZ2	1:A:318:LYS:HB3	1.54	0.73
1:A:227:GLU:C	1:A:228:VAL:HG23	2.14	0.72
1:A:123:ARG:HB2	1:A:144:THR:CG2	2.19	0.72
1:A:144:THR:HG23	1:A:158:ARG:HH12	1.52	0.72
1:A:60:SER:O	1:A:61:PHE:HB2	1.89	0.71
1:A:258:GLU:OE1	1:A:412:LYS:HE2	1.91	0.71
1:A:338:PRO:O	1:A:341:ILE:HG12	1.91	0.71
1:A:107:HIS:HD2	1:A:109:PHE:H	1.37	0.70
1:A:425:ASP:OD2	1:A:425:ASP:C	2.34	0.69
1:A:136:GLY:CA	1:A:168:ASP:HB3	2.23	0.69
1:A:277:MET:HE2	1:A:301:LYS:HZ2	1.58	0.68
1:A:300:LYS:HD2	1:A:388:GLN:HE22	1.59	0.67
1:A:121:THR:O	1:A:158:ARG:NH2	2.26	0.67
1:A:61:PHE:CZ	1:A:240:GLY:HA3	2.30	0.66
1:A:364:PRO:O	1:A:368:LEU:HB2	1.94	0.66
1:A:421:CYS:O	1:A:422:HIS:CB	2.43	0.66
1:A:60:SER:C	1:A:62:VAL:H	2.05	0.65
1:A:60:SER:O	1:A:62:VAL:HG23	1.97	0.64
1:A:130:TYR:HD1	1:A:139:GLU:HG2	1.63	0.63
1:A:134:THR:O	1:A:135:GLN:CB	2.47	0.63
1:A:157:VAL:HG11	1:A:202:LEU:HD23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG12	1:A:206:THR:HG23	1.80	0.62
1:A:300:LYS:HD2	1:A:388:GLN:NE2	2.13	0.62
1:A:177:TRP:CH2	2:A:1:251:H21	2.34	0.61
1:A:259:TRP:CG	1:A:260:TYR:H	2.19	0.61
1:A:61:PHE:N	1:A:64:MET:HE3	2.14	0.60
1:A:60:SER:C	1:A:62:VAL:N	2.58	0.59
1:A:321:ASP:O	1:A:325:LEU:CD2	2.50	0.59
1:A:256:ARG:HD3	1:A:262:GLU:OE2	2.03	0.59
1:A:227:GLU:O	1:A:228:VAL:HG23	2.02	0.58
1:A:76:TYR:CE2	1:A:216:LEU:HG	2.39	0.57
1:A:318:LYS:HB3	1:A:318:LYS:NZ	2.18	0.57
1:A:135:GLN:O	1:A:169:LYS:HG3	2.05	0.56
1:A:315:SER:C	1:A:317:GLU:N	2.55	0.56
1:A:256:ARG:HD2	1:A:264:ILE:HD11	1.87	0.56
1:A:236:MET:HE2	1:A:238:ILE:HD11	1.88	0.56
1:A:245:LEU:HD12	1:A:404:TYR:CE1	2.41	0.56
1:A:259:TRP:CD1	1:A:260:TYR:H	2.23	0.56
1:A:334:ALA:O	1:A:336:THR:N	2.34	0.55
1:A:107:HIS:HB3	1:A:110:LEU:HG	1.89	0.54
1:A:218:GLY:C	1:A:232:VAL:HG12	2.33	0.54
1:A:271:ASN:CB	1:A:344:VAL:HG22	2.38	0.53
1:A:81:THR:HA	1:A:87:GLN:O	2.09	0.52
1:A:215:GLN:NE2	3:A:603:HOH:O	2.41	0.52
1:A:271:ASN:HB3	1:A:344:VAL:HG22	1.91	0.52
1:A:422:HIS:O	1:A:422:HIS:CD2	2.63	0.52
1:A:127:LYS:CG	1:A:142:LEU:HD12	2.32	0.52
1:A:80:MET:HG2	1:A:149:ILE:HG12	1.91	0.52
1:A:157:VAL:CG1	1:A:206:THR:HG23	2.40	0.51
1:A:241:ILE:HD13	1:A:406:VAL:HG21	1.93	0.51
1:A:227:GLU:HA	1:A:227:GLU:OE2	1.82	0.51
1:A:422:HIS:CD2	1:A:422:HIS:C	2.88	0.51
1:A:96:GLY:HA3	2:A:1:251:N36	2.25	0.50
1:A:267:ARG:CG	1:A:348:TYR:CD1	2.94	0.50
1:A:315:SER:O	1:A:317:GLU:N	2.42	0.50
1:A:104:ALA:CB	1:A:163:ALA:HB1	2.41	0.50
1:A:132:PRO:HA	1:A:137:LYS:HB3	1.94	0.50
1:A:356:GLN:HG3	1:A:435:PRO:HB2	1.93	0.49
1:A:227:GLU:C	1:A:228:VAL:HG22	2.35	0.49
1:A:296:LEU:HD22	1:A:399:ILE:HD11	1.94	0.49
1:A:129:VAL:HG13	1:A:129:VAL:O	2.13	0.48
1:A:131:VAL:HG13	1:A:190:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HE3	3:A:581:HOH:O	2.12	0.48
1:A:61:PHE:HZ	1:A:240:GLY:HA3	1.75	0.48
1:A:319:PHE:HB3	1:A:320:PRO:HD2	1.95	0.48
1:A:216:LEU:O	1:A:401:GLU:HA	2.14	0.48
1:A:80:MET:HE1	1:A:181:LEU:HD13	1.95	0.47
1:A:109:PHE:CE1	1:A:173:ASN:ND2	2.83	0.47
1:A:92:LEU:HD23	1:A:180:ILE:HG12	1.97	0.47
1:A:131:VAL:HG21	1:A:138:TRP:CZ2	2.49	0.47
1:A:321:ASP:C	1:A:325:LEU:HD23	2.38	0.47
1:A:412:LYS:HD3	3:A:558:HOH:O	2.14	0.47
1:A:329:LEU:H	1:A:329:LEU:HD23	1.79	0.47
1:A:402:GLY:C	1:A:419:SER:HB2	2.40	0.47
1:A:157:VAL:HG12	1:A:206:THR:CG2	2.45	0.47
1:A:217:CYS:HB2	1:A:233:GLY:O	2.15	0.47
1:A:297:ARG:HB3	1:A:389:SER:HB2	1.97	0.46
1:A:145:ASP:OD1	1:A:146:LEU:N	2.48	0.46
1:A:329:LEU:HD23	1:A:329:LEU:N	2.31	0.46
1:A:267:ARG:HG2	1:A:348:TYR:CD1	2.51	0.46
1:A:284:TYR:O	1:A:285:ASP:CB	2.64	0.46
1:A:336:THR:O	1:A:337:THR:C	2.58	0.45
1:A:422:HIS:O	1:A:422:HIS:HD2	1.99	0.45
1:A:412:LYS:HE3	1:A:412:LYS:HB2	1.62	0.45
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.84	0.45
1:A:130:TYR:CD1	1:A:139:GLU:HG2	2.49	0.45
1:A:267:ARG:HG3	1:A:348:TYR:CD1	2.52	0.45
1:A:296:LEU:HD13	1:A:399:ILE:HG13	1.99	0.44
1:A:425:ASP:OD2	1:A:426:GLU:N	2.49	0.44
1:A:218:GLY:O	1:A:232:VAL:HA	2.17	0.44
1:A:228:VAL:HG23	3:A:595:HOH:O	2.16	0.44
1:A:267:ARG:HG2	1:A:348:TYR:CG	2.52	0.44
1:A:250:LEU:HD23	1:A:417:ALA:HB2	2.00	0.44
1:A:64:MET:CG	1:A:152:GLY:HA2	2.38	0.44
1:A:116:ARG:HG2	1:A:122:TYR:CD1	2.52	0.44
1:A:241:ILE:HD11	1:A:406:VAL:HG11	1.99	0.44
1:A:270:ILE:HB	1:A:309:SER:OG	2.18	0.44
1:A:360:ILE:HA	1:A:431:ALA:O	2.18	0.44
1:A:144:THR:CG2	1:A:158:ARG:HH11	2.21	0.44
1:A:362:ILE:O	1:A:362:ILE:HG13	2.13	0.44
1:A:362:ILE:HD13	1:A:399:ILE:HD13	2.00	0.44
1:A:133:TYR:O	1:A:135:GLN:N	2.51	0.43
1:A:254:PRO:HG2	1:A:350:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:H	1:A:228:VAL:HG22	1.83	0.43
1:A:254:PRO:CG	1:A:350:MET:HE3	2.48	0.43
1:A:115:GLN:NE2	1:A:117:GLN:NE2	2.67	0.43
1:A:300:LYS:HA	1:A:388:GLN:HG3	2.00	0.43
1:A:134:THR:HG21	3:A:514:HOH:O	2.17	0.42
1:A:231:SER:HB2	3:A:592:HOH:O	2.20	0.42
1:A:259:TRP:CG	1:A:260:TYR:N	2.86	0.42
1:A:332:TRP:CE2	1:A:338:PRO:CD	3.03	0.41
1:A:385:ALA:HB1	1:A:398:VAL:HG11	2.00	0.41
1:A:155:VAL:HG11	1:A:206:THR:HB	2.02	0.41
1:A:82:VAL:HG11	1:A:161:ILE:HD13	2.03	0.41
1:A:137:LYS:HG3	1:A:168:ASP:HB2	2.03	0.41
1:A:205:GLN:C	1:A:206:THR:O	2.59	0.41
1:A:399:ILE:O	1:A:403:PHE:HD1	2.04	0.41
1:A:338:PRO:O	1:A:339:TRP:C	2.63	0.41
1:A:408:ASP:CG	1:A:411:ARG:HB2	2.45	0.41
1:A:92:LEU:HB3	1:A:180:ILE:CG1	2.51	0.41
1:A:177:TRP:HH2	2:A:1:251:H21	1.82	0.41
1:A:214:LEU:CD2	1:A:236:MET:HG3	2.51	0.41
1:A:360:ILE:O	1:A:360:ILE:HG13	2.21	0.41
1:A:133:TYR:CE1	1:A:137:LYS:HA	2.56	0.41
1:A:115:GLN:NE2	1:A:117:GLN:HE21	2.20	0.40
1:A:175:SER:O	1:A:176:ASN:CB	2.68	0.40
1:A:227:GLU:N	1:A:228:VAL:HG22	2.36	0.40
1:A:419:SER:HB3	1:A:421:CYS:O	2.21	0.40
1:A:88:THR:O	1:A:89:LEU:HD23	2.21	0.40
1:A:211:LEU:HD23	1:A:212:PHE:N	2.37	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	352/415 (85%)	317 (90%)	20 (6%)	15 (4%)	2 2

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	GLU
1	A	228	VAL
1	A	285	ASP
1	A	335	GLY
1	A	127	LYS
1	A	134	THR
1	A	135	GLN
1	A	271	ASN
1	A	339	TRP
1	A	126	ARG
1	A	354	THR
1	A	427	PHE
1	A	210	ASN
1	A	316	THR
1	A	337	THR

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	307/356 (86%)	262 (85%)	45 (15%)	3 6

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	63	GLU
1	A	65	VAL
1	A	69	ARG
1	A	108	PRO
1	A	134	THR

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Mol	Chain	Res	Type
1	A	137	LYS
1	A	148	SER
1	A	155	VAL
1	A	168	ASP
1	A	169	LYS
1	A	172	ILE
1	A	180	ILE
1	A	202	LEU
1	A	216	LEU
1	A	227	GLU
1	A	228	VAL
1	A	231	SER
1	A	241	ILE
1	A	244	SER
1	A	249	SER
1	A	259	TRP
1	A	267	ARG
1	A	271	ASN
1	A	318	LYS
1	A	319	PHE
1	A	327	GLU
1	A	329	LEU
1	A	331	CYS
1	A	337	THR
1	A	347	LEU
1	A	355	ASN
1	A	356	GLN
1	A	357	SER
1	A	362	ILE
1	A	368	LEU
1	A	371	VAL
1	A	380	ASP
1	A	390	SER
1	A	391	THR
1	A	401	GLU
1	A	422	HIS
1	A	425	ASP
1	A	426	GLU
1	A	443	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	115	GLN
1	A	117	GLN
1	A	160	ASN
1	A	173	ASN
1	A	215	GLN
1	A	328	GLN
1	A	388	GLN

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 ⓘ

There are no oligosaccharides 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	251	A	1	-	26,26,26	2.91	17 (65%)	33,35,35	1.24	6 (18%)

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	251	A	1	-	-	0/16/16/16	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	251	C18-C17	5.15	1.47	1.39
2	A	1	251	C12-N16	4.90	1.50	1.40
2	A	1	251	C15-N16	4.81	1.49	1.40
2	A	1	251	C22-C17	4.02	1.45	1.39
2	A	1	251	C2-C3	3.68	1.45	1.39
2	A	1	251	C1-C2	3.67	1.45	1.38
2	A	1	251	C28-N16	3.56	1.51	1.46
2	A	1	251	C6-C1	3.31	1.45	1.38
2	A	1	251	C19-C18	3.10	1.44	1.38
2	A	1	251	C5-C4	2.99	1.44	1.38
2	A	1	251	C6-C5	2.92	1.44	1.38
2	A	1	251	C4-C3	2.89	1.43	1.39
2	A	1	251	C20-C19	2.81	1.44	1.38
2	A	1	251	C21-C22	2.66	1.43	1.38
2	A	1	251	C17-C15	2.41	1.51	1.48
2	A	1	251	C14-C13	2.41	1.47	1.39
2	A	1	251	C21-C20	2.23	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	251	C3-C12-N16	2.61	127.72	123.19
2	A	1	251	C17-C15-N16	2.51	127.55	123.19
2	A	1	251	C14-C13-C12	2.41	109.96	107.48
2	A	1	251	C13-C14-C15	2.36	109.91	107.48
2	A	1	251	C29-C28-N16	-2.12	107.07	111.52
2	A	1	251	C28-N16-C12	2.07	128.39	125.73

There are no chirality outliers.

There are no torsion outliers.

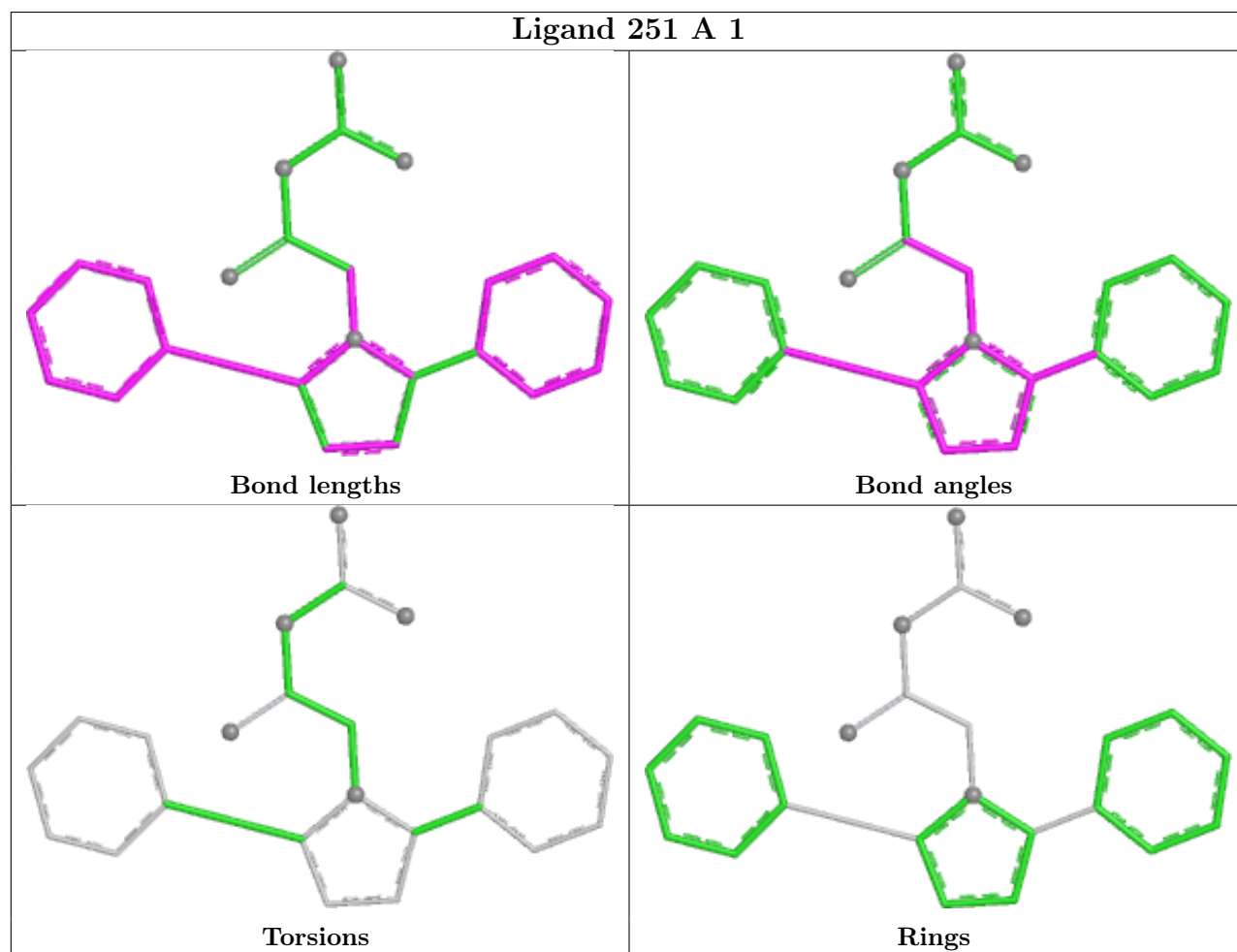
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	251	3	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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.