Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 06:55 AM EDT

PDB ID	:	2QU2
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:

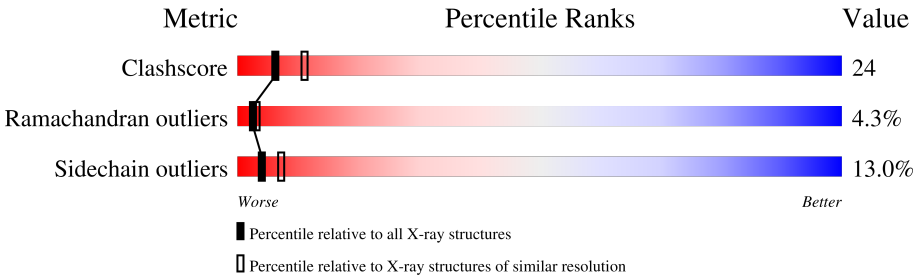
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	415	50% 30% 7% • 12%

2 Entry composition

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.

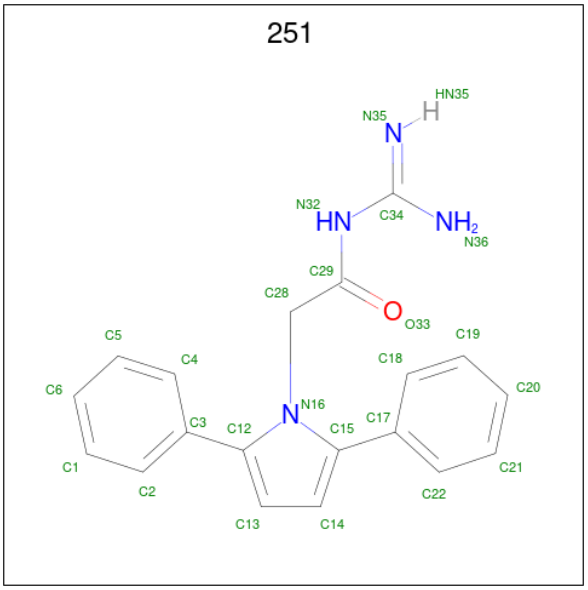
- Molecule 1 is a protein called Beta-secretase 1.

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

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 (three-letter code: 251) (formula: $C_{19}H_{18}N_4O$).



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		

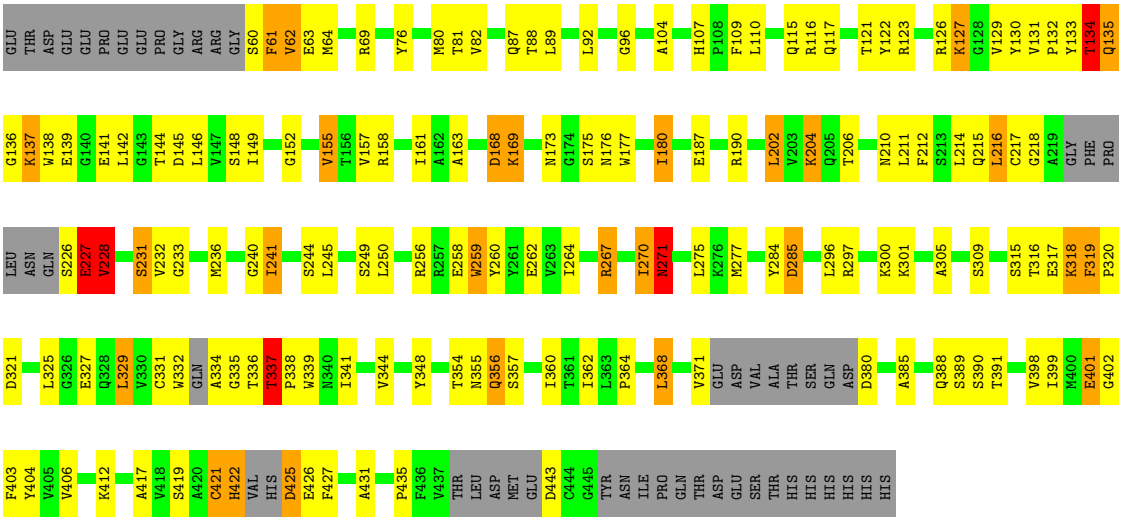
3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

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	0.50	2/2923 (0.1%)	0.85	10/3966 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	ASN	CB-CG	8.93	1.71	1.51
1	A	271	ASN	C-O	5.72	1.34	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	226	SER	C-N-CA	7.25	139.82	121.70
1	A	271	ASN	CA-C-N	-6.85	102.51	116.20
1	A	227	GLU	CA-CB-CG	-6.43	99.26	113.40
1	A	270	ILE	CA-C-N	-6.32	103.30	117.20
1	A	271	ASN	N-CA-C	5.87	126.86	111.00
1	A	227	GLU	N-CA-CB	5.86	121.15	110.60
1	A	141	GLU	N-CA-C	-5.41	96.39	111.00
1	A	61	PHE	N-CA-C	-5.35	96.56	111.00
1	A	270	ILE	N-CA-C	-5.14	97.12	111.00
1	A	421	CYS	CA-CB-SG	-5.11	104.80	114.00

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	2854	0	2777	138	0
2	A	24	0	18	3	0
3	A	156	0	0	6	0
All	All	3034	0	2795	138	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 24.

All (138) 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: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: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:136:GLY:HA2	1:A:168:ASP:HB3	1.64	0.80
1:A:315:SER:C	1:A:317:GLU:H	1.85	0.80
1:A:227:GLU:C	1:A:228:VAL:CG2	2.53	0.76
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: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:136:GLY:CA	1:A:168:ASP:HB3	2.23	0.69
1:A:227:GLU:C	1:A:228:VAL:HG23	2.14	0.68
1:A:318:LYS:HZ2	1:A:318:LYS:HB3	1.60	0.67
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:CYS:O	1:A:422:HIS:CB	2.43	0.66
1:A:425:ASP:OD2	1:A:425:ASP:C	2.34	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
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:60:SER:C	1:A:62:VAL:H	2.05	0.60
1:A:277:MET:HE1	1:A:301:LYS:HG2	1.83	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:60:SER:C	1:A:62:VAL:N	2.58	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:256:ARG:HD2	1:A:264:ILE:HD11	1.87	0.56
1:A:245:LEU:HD12	1:A:404:TYR:CE1	2.41	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: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: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:315:SER:C	1:A:317:GLU:N	2.55	0.49
1:A:356:GLN:HG3	1:A:435:PRO:HB2	1.93	0.49
1:A:362:ILE:O	1:A:362:ILE:HG13	2.13	0.49
1:A:218:GLY:C	1:A:232:VAL:HG12	2.33	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:277:MET:HE3	1:A:305:ALA:HB2	1.97	0.46
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:422:HIS:CD2	1:A:422:HIS:C	2.88	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: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:277:MET:HE3	1:A:305:ALA:CB	2.48	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:227:GLU:C	1:A:228:VAL:HG22	2.35	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:HD13	1:A:399:ILE:HD13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:O	1:A:135:GLN:N	2.51	0.43
1:A:227:GLU:H	1:A:228:VAL:HG22	1.83	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:61:PHE:H	1:A:64:MET:CE	2.32	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:402:GLY:C	1:A:419:SER:HB2	2.40	0.42
1:A:332:TRP:CE2	1:A:338:PRO:CD	3.03	0.41
1:A:336:THR:O	1:A:337:THR:C	2.58	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:399:ILE:O	1:A:403:PHE:HD1	2.04	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
1:A:321:ASP:C	1:A:325:LEU:HD23	2.38	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	352/415 (85%)	317 (90%)	20 (6%)	15 (4%)	2 3

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 (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	307/356 (86%)	267 (87%)	40 (13%)	4 7

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	63	GLU
1	A	69	ARG
1	A	134	THR
1	A	137	LYS
1	A	148	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	155	VAL
1	A	168	ASP
1	A	169	LYS
1	A	180	ILE
1	A	187	GLU
1	A	202	LEU
1	A	204	LYS
1	A	216	LEU
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	355	ASN
1	A	356	GLN
1	A	357	SER
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	443	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	115	GLN
1	A	173	ASN
1	A	215	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	273	GLN
1	A	328	GLN
1	A	388	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	-	21,26,26	2.30	10 (47%)	21,35,35	0.62	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	251	A	1	-	-	0/8/16/16	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	251	C1-C2	4.04	1.45	1.36
2	A	1	251	C19-C18	3.56	1.44	1.36
2	A	1	251	C5-C4	3.47	1.44	1.36
2	A	1	251	C6-C1	3.31	1.45	1.38
2	A	1	251	C21-C22	3.20	1.43	1.36
2	A	1	251	C6-C5	2.92	1.44	1.38
2	A	1	251	C20-C19	2.81	1.44	1.38
2	A	1	251	C14-C13	2.80	1.47	1.38
2	A	1	251	C18-C17	2.40	1.47	1.42
2	A	1	251	C21-C20	2.23	1.43	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

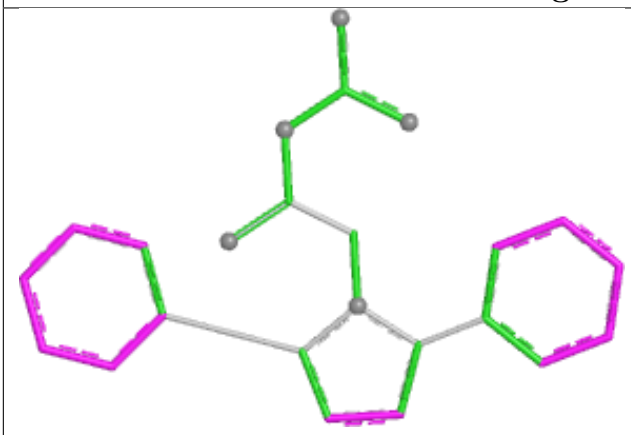
There are no ring outliers.

1 monomer is involved in 3 short contacts:

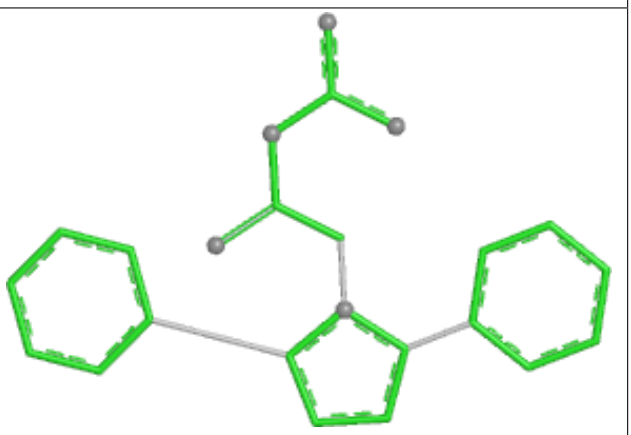
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	251	3	0

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 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.

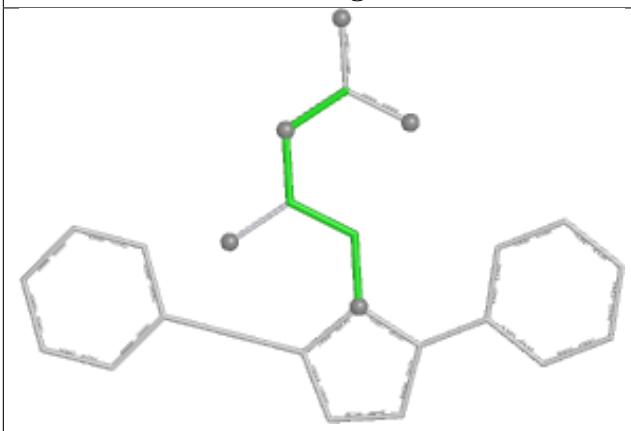
Ligand 251 A 1



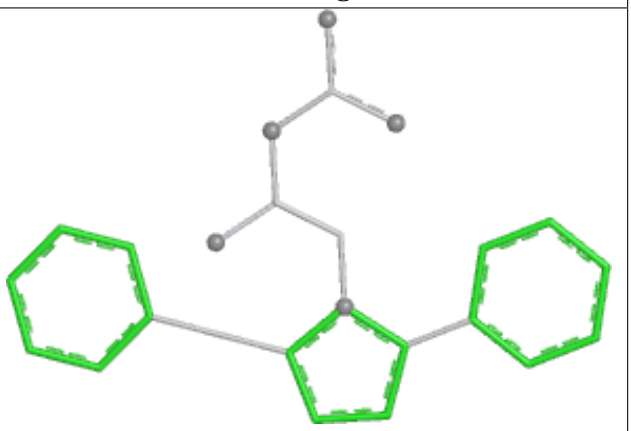
Bond lengths



Bond angles



Torsions



Rings

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.