



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 02:22 AM EDT

PDB ID : 5DQC  
Title : Co-crystal of BACE1 with compound 0211  
Authors : Ghosh, A.K.; Bhavanam, S.R.; Yen, T.-C.; Cardenas, E.L.; Rao, K.V.; Downs, D.; Huang, X.; Tang, J.; Mescar, A.D.  
Deposited on : 2015-09-14  
Resolution : 2.47 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

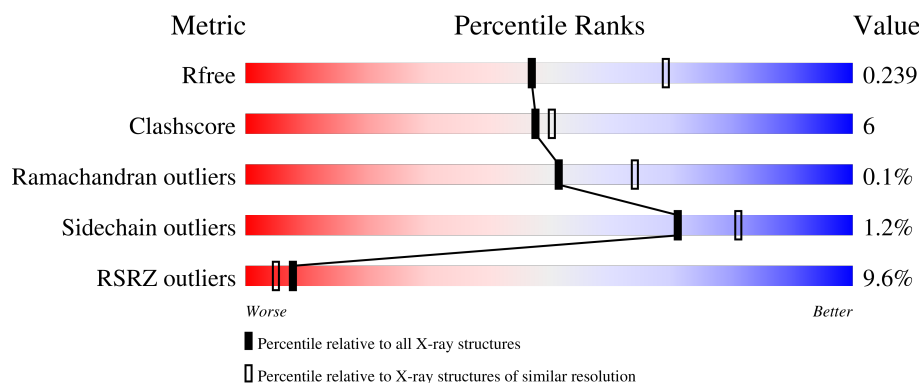
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.47 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))
$R_{free}$	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 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	390	<div> <div>6%</div> <div>83%</div> <div>12%</div> <div>• 5%</div> </div>
1	B	390	<div> <div>14%</div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div>
1	C	390	<div> <div>7%</div> <div>85%</div> <div>11%</div> <div>•</div> </div>

## 2 Entry composition [i](#)

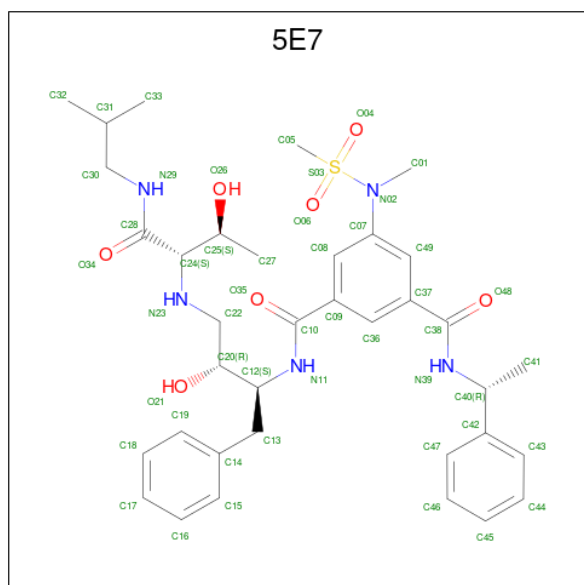
There are 3 unique types of molecules in this entry. The entry contains 9054 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	372	Total	C	N	O	S	2	0	0
			2929	1877	488	550	14			
1	B	369	Total	C	N	O	S	10	0	0
			2910	1868	484	544	14			
1	C	373	Total	C	N	O	S	4	0	0
			2940	1882	489	555	14			

- Molecule 2 is N-[(2S,3R)-3-hydroxy-4-({(2S,3S)-3-hydroxy-1-[(2-methylpropyl)amino]-1-oxobutan-2-yl}amino)-1-phenylbutan-2-yl]-5-[methyl(methylsulfonyl)amino]-N'-[(1R)-1-phenylethyl]benzene-1,3-dicarboxamide (three-letter code: 5E7) (formula: C<sub>36</sub>H<sub>49</sub>N<sub>5</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			49	36	5	7	1		
2	B	1	Total	C	N	O	S	0	0
			49	36	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			49	36	5	7	1		

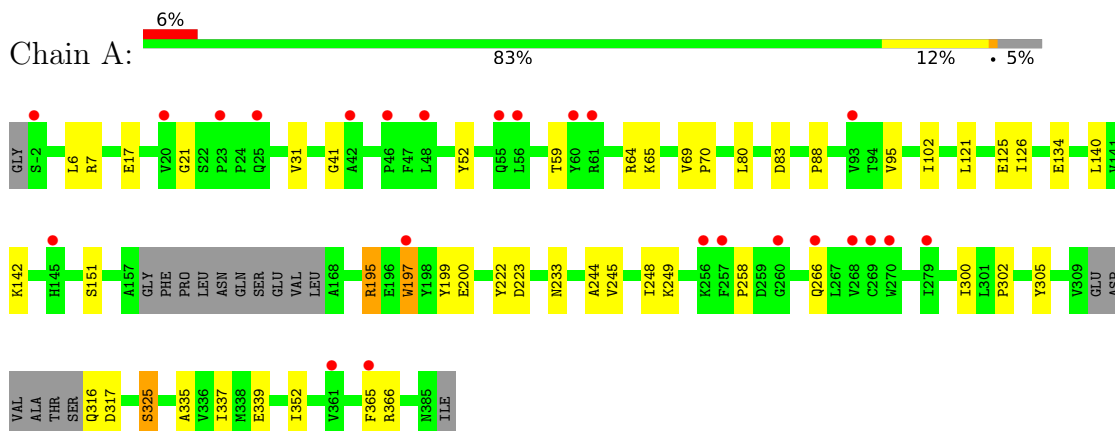
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	35	Total	O	0	0
			35	35		
3	C	46	Total	O	0	0
			46	46		

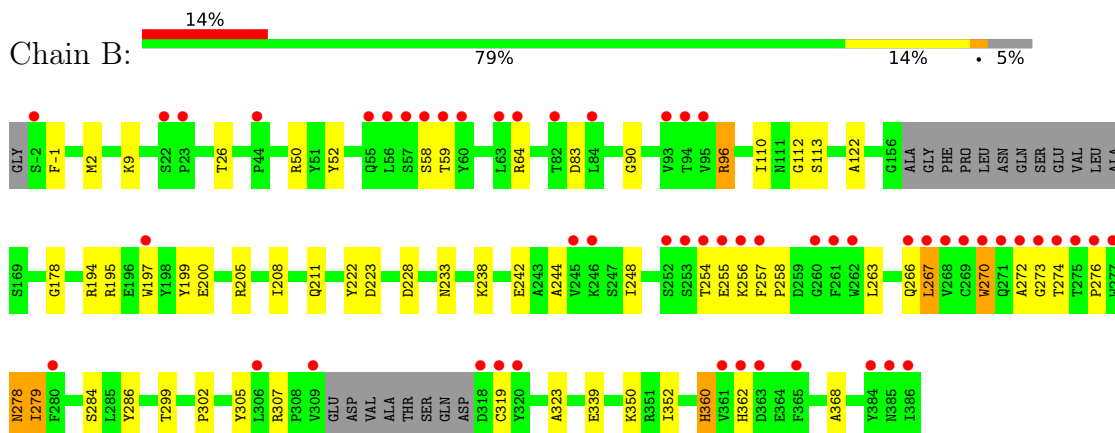
### 3 Residue-property plots [i](#)

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 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.

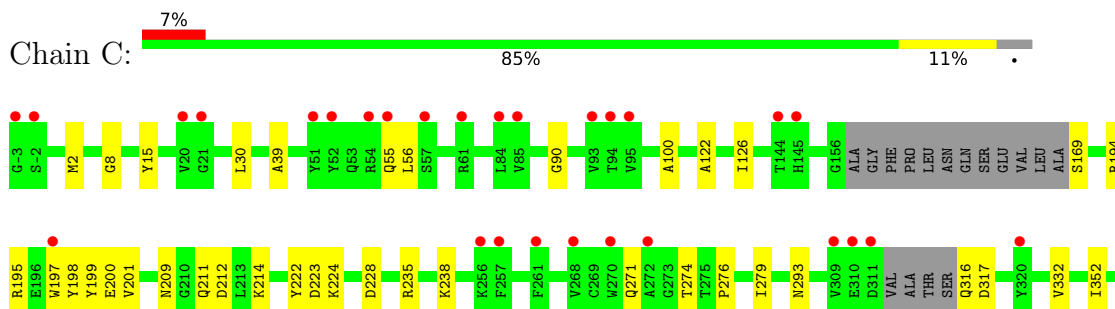
#### • Molecule 1: Beta-secretase 1

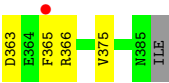


#### • Molecule 1: Beta-secretase 1



#### • Molecule 1: Beta-secretase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.95Å 103.40Å 100.83Å 90.00° 102.66° 90.00°	Depositor
Resolution (Å)	45.77 – 2.47 45.77 – 2.47	Depositor EDS
% Data completeness (in resolution range)	89.3 (45.77-2.47) 84.3 (45.77-2.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.54 (at 2.45Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.185 , 0.235 0.193 , 0.239	Depositor DCC
$R_{free}$ test set	2000 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 5E7

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	0.28	0/3003	0.48	1/4079 (0.0%)
1	B	0.30	1/2984 (0.0%)	0.52	1/4053 (0.0%)
1	C	0.29	0/3014	0.49	0/4093
All	All	0.29	1/9001 (0.0%)	0.50	2/12225 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	TRP	CB-CG	5.29	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	267	LEU	CA-CB-CG	5.01	126.82	115.30

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	2929	0	2846	30	0
1	B	2910	0	2835	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2940	0	2849	37	0
2	A	49	0	49	0	0
2	B	49	0	49	4	0
2	C	49	0	49	2	0
3	A	47	0	0	2	1
3	B	35	0	0	1	0
3	C	46	0	0	5	1
All	All	9054	0	8677	108	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 6.

All (108) 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:C:195:ARG:HB3	1:C:197:TRP:HZ3	1.36	0.91
1:B:59:THR:O	1:B:96:ARG:NH2	2.09	0.86
1:A:134:GLU:OE1	3:A:501:HOH:O	1.95	0.83
1:B:122:ALA:O	3:B:501:HOH:O	2.02	0.77
1:C:169:SER:OG	3:C:501:HOH:O	1.96	0.75
1:A:258:PRO:HB2	1:A:266:GLN:HE22	1.52	0.74
1:C:212:ASP:OD2	3:C:502:HOH:O	2.09	0.70
1:B:258:PRO:CG	1:B:266:GLN:HE21	2.05	0.69
1:C:316:GLN:HG3	1:C:317:ASP:H	1.58	0.69
1:B:270:TRP:HB3	1:B:274:THR:HG23	1.75	0.67
1:A:195:ARG:HB3	1:A:197:TRP:CZ3	2.31	0.65
1:A:6:LEU:O	1:A:7:ARG:NH1	2.29	0.64
1:A:316:GLN:HG3	1:A:317:ASP:N	2.15	0.62
1:C:195:ARG:HB3	1:C:197:TRP:CZ3	2.28	0.61
1:C:197:TRP:CD1	1:C:198:TYR:CD2	2.89	0.60
1:A:245:VAL:HG12	1:A:249:LYS:HD2	1.84	0.60
1:B:195:ARG:HB3	1:B:197:TRP:CZ3	2.38	0.59
1:A:233:ASN:ND2	1:A:325:SER:OG	2.27	0.59
1:B:199:TYR:HB3	1:B:352:ILE:HD11	1.83	0.59
1:C:55:GLN:HB2	1:C:56:LEU:HD13	1.85	0.59
1:A:95:VAL:HG11	1:A:140:LEU:HA	1.85	0.59
2:B:401:5E7:H4	2:B:401:5E7:C49	2.33	0.59
1:C:126:ILE:HG23	1:C:197:TRP:HB2	1.85	0.57
1:B:284:SER:HG	1:B:299:THR:HG1	1.44	0.57
1:C:271:GLN:O	1:C:274:THR:OG1	2.17	0.56
1:B:276:PRO:HB2	1:B:279:ILE:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LYS:O	1:B:242:GLU:HG2	2.07	0.55
1:C:228:ASP:OD2	2:C:401:5E7:N23	2.39	0.55
1:A:134:GLU:OE2	1:A:142:LYS:NZ	2.30	0.54
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.89	0.54
1:B:195:ARG:HB3	1:B:197:TRP:HZ3	1.72	0.54
1:B:258:PRO:HG3	1:B:266:GLN:HE21	1.72	0.54
1:B:360:HIS:CE1	1:B:362:HIS:HB3	2.43	0.54
1:B:360:HIS:CE1	1:B:368:ALA:H	2.26	0.53
1:B:233:ASN:H	2:B:401:5E7:H5	1.74	0.53
2:B:401:5E7:H4	2:B:401:5E7:H48	1.91	0.52
1:A:125:GLU:HG2	1:A:197:TRP:HB3	1.92	0.52
1:C:293:ASN:HA	1:C:375:VAL:HA	1.91	0.51
1:A:199:TYR:HB3	1:A:352:ILE:HD11	1.92	0.51
1:B:267:LEU:HD23	1:B:319:CYS:HB3	1.91	0.51
1:C:209:ASN:OD1	3:C:503:HOH:O	2.19	0.51
1:B:110:ILE:HB	1:B:113:SER:HB3	1.92	0.51
1:B:270:TRP:HB3	1:B:274:THR:CG2	2.38	0.51
1:C:197:TRP:HH2	1:C:200:GLU:OE1	1.94	0.51
1:A:258:PRO:HB2	1:A:266:GLN:NE2	2.24	0.50
1:C:316:GLN:HG3	1:C:317:ASP:N	2.26	0.49
1:C:211:GLN:HG3	3:C:538:HOH:O	2.12	0.49
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.95	0.49
1:B:276:PRO:HA	1:B:278:ASN:HD22	1.76	0.49
1:A:197:TRP:HH2	1:A:200:GLU:OE1	1.95	0.48
1:A:17:GLU:HG2	1:A:88:PRO:HG2	1.95	0.48
1:C:197:TRP:NE1	1:C:198:TYR:HD2	2.12	0.48
1:C:199:TYR:HB3	1:C:352:ILE:HD11	1.94	0.48
1:C:365:PHE:CD1	1:C:366:ARG:HG3	2.49	0.48
1:A:126:ILE:HG23	1:A:197:TRP:HB2	1.95	0.48
1:C:200:GLU:HG2	1:C:201:VAL:N	2.28	0.47
1:B:307:ARG:HG3	1:B:323:ALA:HB2	1.96	0.47
1:C:198:TYR:HB3	3:C:517:HOH:O	2.15	0.47
1:C:214:LYS:HB3	1:C:214:LYS:HE3	1.62	0.47
1:B:194:ARG:HD3	1:B:200:GLU:OE1	2.15	0.47
1:B:307:ARG:NH2	1:B:339:GLU:OE2	2.47	0.46
1:C:235:ARG:HB2	1:C:332:VAL:HB	1.98	0.46
1:B:9:LYS:HE3	1:B:112:GLY:O	2.16	0.46
1:C:198:TYR:CE2	1:C:224:LYS:HE3	2.51	0.46
1:B:244:ALA:O	1:B:248:ILE:HG13	2.16	0.46
1:B:302:PRO:HA	1:B:305:TYR:CZ	2.51	0.46
1:C:197:TRP:CG	1:C:198:TYR:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLN:HG3	1:A:317:ASP:H	1.80	0.46
1:A:300:ILE:HG21	1:A:337:ILE:HD13	1.99	0.45
1:B:256:LYS:HD2	1:B:257:PHE:H	1.80	0.45
1:B:254:THR:OG1	1:B:279:ILE:HD12	2.17	0.45
1:B:-1:PHE:CZ	1:B:178:GLY:HA3	2.51	0.45
1:B:350:LYS:HE2	1:B:350:LYS:HB3	1.75	0.45
1:C:363:ASP:HB3	1:C:366:ARG:O	2.17	0.44
1:B:208:ILE:O	1:B:211:GLN:HB3	2.17	0.44
1:B:222:TYR:HA	1:B:223:ASP:HA	1.63	0.44
1:B:238:LYS:H	1:B:238:LYS:HG3	1.41	0.44
1:A:365:PHE:CD1	1:A:366:ARG:HG3	2.52	0.44
1:B:52:TYR:OH	1:B:83:ASP:OD2	2.29	0.44
1:B:272:ALA:HA	1:B:273:GLY:HA2	1.62	0.44
1:C:195:ARG:CB	1:C:197:TRP:HZ3	2.20	0.44
1:C:222:TYR:HA	1:C:223:ASP:HA	1.65	0.43
1:A:52:TYR:OH	1:A:83:ASP:OD2	2.33	0.43
1:A:21:GLY:HA2	1:A:83:ASP:OD1	2.19	0.43
1:A:244:ALA:O	1:A:248:ILE:HD12	2.19	0.43
1:C:197:TRP:CH2	1:C:200:GLU:OE1	2.71	0.43
1:A:222:TYR:HA	1:A:223:ASP:HA	1.67	0.42
1:C:8:GLY:HA2	1:C:15:TYR:CE2	2.55	0.42
1:C:197:TRP:HE1	1:C:198:TYR:HD2	1.68	0.42
1:C:194:ARG:HD3	1:C:200:GLU:OE1	2.20	0.42
1:C:238:LYS:HB2	1:C:238:LYS:HE2	1.83	0.42
1:A:65:LYS:HB3	1:A:80:LEU:HD12	2.02	0.42
1:A:335:ALA:O	1:A:339:GLU:HG3	2.20	0.42
1:A:41:GLY:HA2	1:A:102:ILE:HB	2.02	0.42
1:A:17:GLU:O	1:A:88:PRO:HD2	2.20	0.41
1:B:26:THR:O	1:B:50:ARG:NH1	2.54	0.41
1:C:30:LEU:HD22	2:C:401:5E7:H12	2.01	0.41
1:A:69:VAL:HA	1:A:70:PRO:HD3	1.89	0.41
1:A:31:VAL:HG13	1:A:121:LEU:HD11	2.03	0.41
1:A:200:GLU:OE2	3:A:502:HOH:O	2.22	0.41
1:B:205:ARG:HB2	1:B:286:TYR:HB2	2.03	0.41
1:B:256:LYS:HD2	1:B:256:LYS:HA	1.74	0.41
1:C:276:PRO:O	1:C:279:ILE:HG12	2.21	0.41
1:C:122:ALA:HB1	1:C:197:TRP:O	2.21	0.40
1:B:228:ASP:OD2	2:B:401:5E7:H20	2.22	0.40
1:B:254:THR:OG1	1:B:255:GLU:N	2.54	0.40
1:C:39:ALA:HB2	1:C:100:ALA:HB3	2.04	0.40
1:A:302:PRO:HA	1:A:305:TYR:CE2	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)
3:A:525:HOH:O	3:C:544:HOH:O[2_646]	1.90	0.30

## 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	366/390 (94%)	360 (98%)	6 (2%)	0	100	100
1	B	363/390 (93%)	346 (95%)	16 (4%)	1 (0%)	41	49
1	C	367/390 (94%)	355 (97%)	12 (3%)	0	100	100
All	All	1096/1170 (94%)	1061 (97%)	34 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	278	ASN

### 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	317/332 (96%)	312 (98%)	5 (2%)	62	74
1	B	316/332 (95%)	310 (98%)	6 (2%)	57	69
1	C	319/332 (96%)	319 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	952/996 (96%)	941 (99%)	11 (1%)	71	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	THR
1	A	64	ARG
1	A	151	SER
1	A	197	TRP
1	A	325	SER
1	B	58	SER
1	B	64	ARG
1	B	96	ARG
1	B	263	LEU
1	B	279	ILE
1	B	360	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	B	266	GLN
1	B	278	ASN
1	B	360	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 ⓘ

There are no monosaccharides 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	5E7	A	401	-	50,51,51	1.34	6 (12%)	66,71,71	1.80	19 (28%)
2	5E7	B	401	-	50,51,51	1.45	7 (14%)	66,71,71	1.87	18 (27%)
2	5E7	C	401	-	50,51,51	1.44	7 (14%)	66,71,71	1.75	18 (27%)

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	5E7	A	401	-	-	12/56/56/56	0/3/3/3
2	5E7	B	401	-	-	21/56/56/56	0/3/3/3
2	5E7	C	401	-	-	10/56/56/56	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	5E7	S03-N02	4.65	1.74	1.64
2	A	401	5E7	C22-C20	3.60	1.57	1.52
2	C	401	5E7	S03-N02	3.25	1.71	1.64
2	C	401	5E7	C28-N29	3.23	1.40	1.33
2	C	401	5E7	C20-C12	3.15	1.59	1.53
2	B	401	5E7	C28-N29	3.07	1.40	1.33
2	C	401	5E7	C38-N39	3.03	1.40	1.34
2	B	401	5E7	C10-N11	3.00	1.40	1.34
2	A	401	5E7	S03-N02	2.97	1.71	1.64
2	B	401	5E7	C38-N39	2.92	1.40	1.34
2	A	401	5E7	C20-C12	2.88	1.58	1.53
2	C	401	5E7	C24-C28	2.82	1.60	1.52
2	A	401	5E7	C28-N29	2.78	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	5E7	C22-C20	2.65	1.56	1.52
2	A	401	5E7	C38-N39	2.56	1.39	1.34
2	C	401	5E7	C10-N11	2.55	1.39	1.34
2	B	401	5E7	C24-C28	2.39	1.59	1.52
2	A	401	5E7	C10-N11	2.36	1.39	1.34
2	B	401	5E7	C22-C20	2.28	1.55	1.52
2	B	401	5E7	C08-C07	2.12	1.43	1.39

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	5E7	C12-N11-C10	4.85	131.84	123.01
2	A	401	5E7	C24-C28-N29	4.82	124.72	116.41
2	C	401	5E7	C40-N39-C38	4.78	132.94	122.56
2	C	401	5E7	C12-N11-C10	4.71	131.59	123.01
2	A	401	5E7	C12-N11-C10	4.70	131.56	123.01
2	B	401	5E7	C37-C49-C07	4.43	124.64	119.59
2	B	401	5E7	C37-C36-C09	4.23	125.37	120.44
2	C	401	5E7	C37-C36-C09	4.10	125.21	120.44
2	B	401	5E7	C40-N39-C38	4.08	131.41	122.56
2	A	401	5E7	C40-N39-C38	3.89	131.00	122.56
2	B	401	5E7	C24-C28-N29	3.88	123.10	116.41
2	C	401	5E7	C24-C28-N29	3.81	122.98	116.41
2	A	401	5E7	C37-C36-C09	3.74	124.80	120.44
2	B	401	5E7	C49-C37-C36	-3.62	115.27	119.63
2	A	401	5E7	C49-C37-C36	-3.43	115.51	119.63
2	C	401	5E7	C49-C37-C36	-3.42	115.51	119.63
2	A	401	5E7	C37-C49-C07	3.37	123.43	119.59
2	C	401	5E7	C37-C49-C07	3.17	123.20	119.59
2	A	401	5E7	O48-C38-N39	-3.04	116.86	122.45
2	C	401	5E7	O06-S03-O04	-3.02	114.28	118.59
2	B	401	5E7	O06-S03-N02	2.95	110.63	107.08
2	B	401	5E7	O35-C10-N11	-2.92	117.08	122.45
2	B	401	5E7	O48-C38-N39	-2.91	117.10	122.45
2	B	401	5E7	C37-C38-N39	2.90	122.63	117.06
2	A	401	5E7	C37-C38-N39	2.87	122.56	117.06
2	A	401	5E7	C09-C10-N11	2.85	122.52	117.06
2	A	401	5E7	O06-S03-N02	2.84	110.50	107.08
2	A	401	5E7	O35-C10-N11	-2.81	117.28	122.45
2	B	401	5E7	C09-C10-N11	2.80	122.43	117.06
2	C	401	5E7	O35-C10-N11	-2.78	117.34	122.45
2	B	401	5E7	O06-S03-O04	-2.73	114.70	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	5E7	C09-C10-N11	2.61	122.07	117.06
2	C	401	5E7	O48-C38-N39	-2.57	117.73	122.45
2	B	401	5E7	C36-C09-C08	-2.53	116.59	119.63
2	B	401	5E7	O34-C28-N29	-2.45	117.74	122.99
2	C	401	5E7	O06-S03-N02	2.42	110.00	107.08
2	C	401	5E7	C36-C09-C08	-2.37	116.78	119.63
2	A	401	5E7	C18-C19-C14	2.33	124.20	120.63
2	A	401	5E7	O34-C28-N29	-2.30	118.05	122.99
2	C	401	5E7	C18-C19-C14	2.30	124.16	120.63
2	A	401	5E7	C36-C09-C08	-2.27	116.89	119.63
2	C	401	5E7	O34-C28-N29	-2.26	118.14	122.99
2	C	401	5E7	C37-C38-N39	2.26	121.39	117.06
2	A	401	5E7	C25-C24-C28	-2.26	106.31	111.28
2	A	401	5E7	O06-S03-O04	-2.23	115.41	118.59
2	A	401	5E7	C19-C14-C15	-2.23	114.66	118.17
2	C	401	5E7	C19-C14-C15	-2.20	114.71	118.17
2	A	401	5E7	C09-C08-C07	2.18	122.08	119.59
2	B	401	5E7	C09-C08-C07	2.18	122.08	119.59
2	B	401	5E7	C18-C19-C14	2.16	123.95	120.63
2	B	401	5E7	C19-C14-C15	-2.10	114.86	118.17
2	C	401	5E7	C09-C08-C07	2.07	121.95	119.59
2	A	401	5E7	C13-C14-C15	2.03	124.93	120.91
2	C	401	5E7	C13-C14-C15	2.02	124.91	120.91
2	B	401	5E7	C13-C14-C15	2.01	124.91	120.91

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	5E7	C08-C07-N02-S03
2	A	401	5E7	C49-C07-N02-S03
2	A	401	5E7	N11-C12-C13-C14
2	A	401	5E7	C25-C24-N23-C22
2	B	401	5E7	C01-N02-S03-O04
2	B	401	5E7	C01-N02-S03-C05
2	B	401	5E7	C07-N02-S03-O04
2	B	401	5E7	C07-N02-S03-C05
2	B	401	5E7	C07-N02-S03-O06
2	B	401	5E7	C08-C07-N02-S03
2	B	401	5E7	C49-C07-N02-S03
2	B	401	5E7	N11-C12-C13-C14
2	B	401	5E7	C28-C24-C25-O26

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Mol	Chain	Res	Type	Atoms
2	B	401	5E7	C28-C24-C25-C27
2	C	401	5E7	C08-C07-N02-S03
2	C	401	5E7	C49-C07-N02-S03
2	C	401	5E7	C25-C24-N23-C22
2	C	401	5E7	C28-C24-N23-C22
2	A	401	5E7	N29-C30-C31-C32
2	B	401	5E7	N29-C30-C31-C32
2	A	401	5E7	N23-C24-C28-O34
2	C	401	5E7	N23-C24-C28-O34
2	A	401	5E7	N23-C24-C28-N29
2	C	401	5E7	N23-C24-C28-N29
2	A	401	5E7	N23-C24-C25-C27
2	B	401	5E7	N23-C24-C25-O26
2	C	401	5E7	N11-C12-C13-C14
2	B	401	5E7	C12-C20-C22-N23
2	A	401	5E7	N23-C24-C25-O26
2	B	401	5E7	N29-C30-C31-C33
2	A	401	5E7	C20-C22-N23-C24
2	B	401	5E7	C20-C22-N23-C24
2	A	401	5E7	N29-C30-C31-C33
2	B	401	5E7	N23-C24-C28-N29
2	C	401	5E7	C12-C13-C14-C19
2	B	401	5E7	N23-C24-C28-O34
2	B	401	5E7	N23-C24-C25-C27
2	C	401	5E7	C12-C13-C14-C15
2	C	401	5E7	C20-C22-N23-C24
2	A	401	5E7	C12-C13-C14-C19
2	B	401	5E7	C20-C12-C13-C14
2	B	401	5E7	C25-C24-N23-C22
2	B	401	5E7	C12-C13-C14-C19

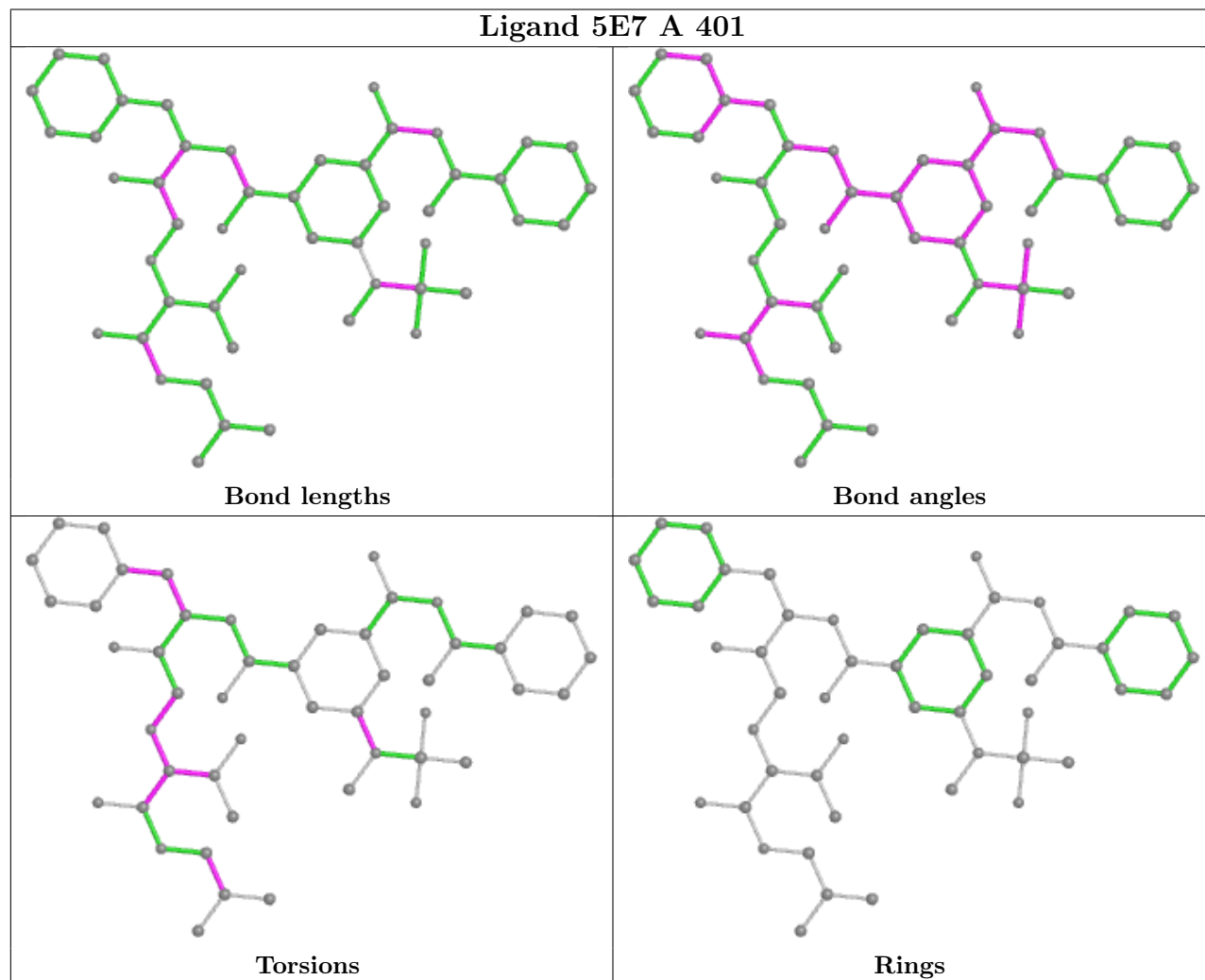
There are no ring outliers.

2 monomers are involved in 6 short contacts:

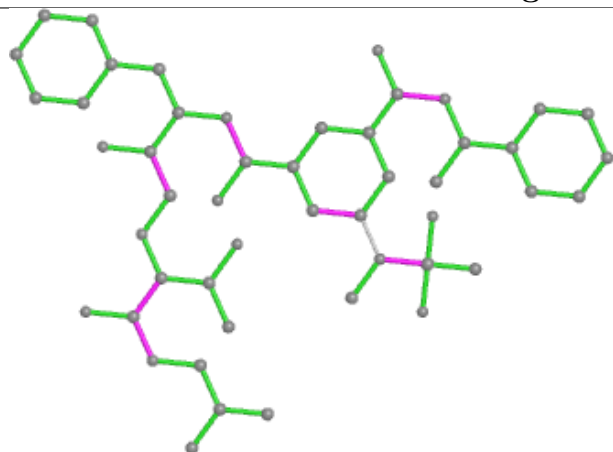
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	5E7	4	0
2	C	401	5E7	2	0

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

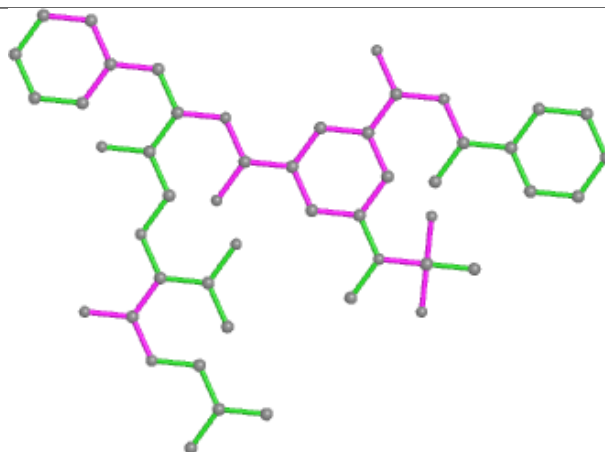
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



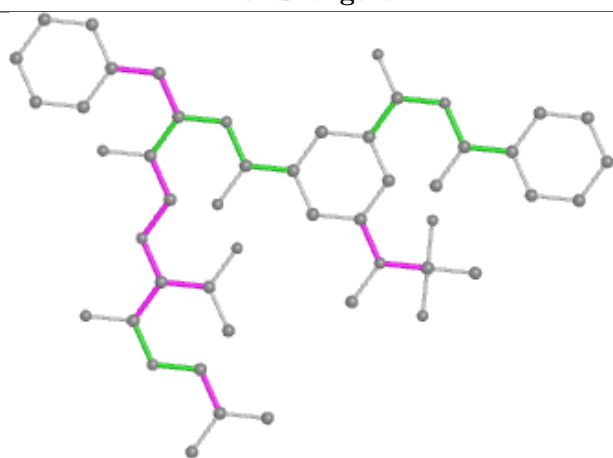
## Ligand 5E7 B 401



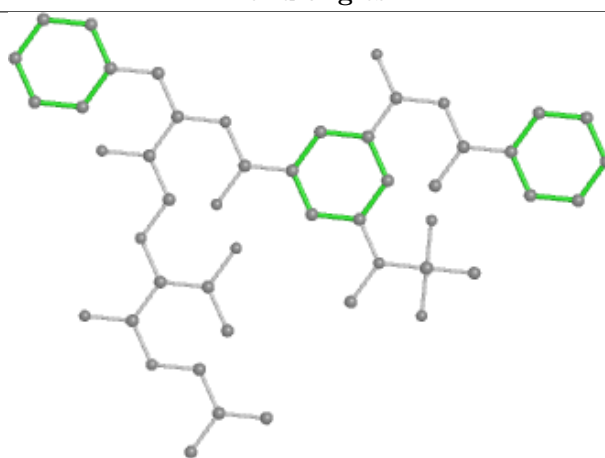
Bond lengths



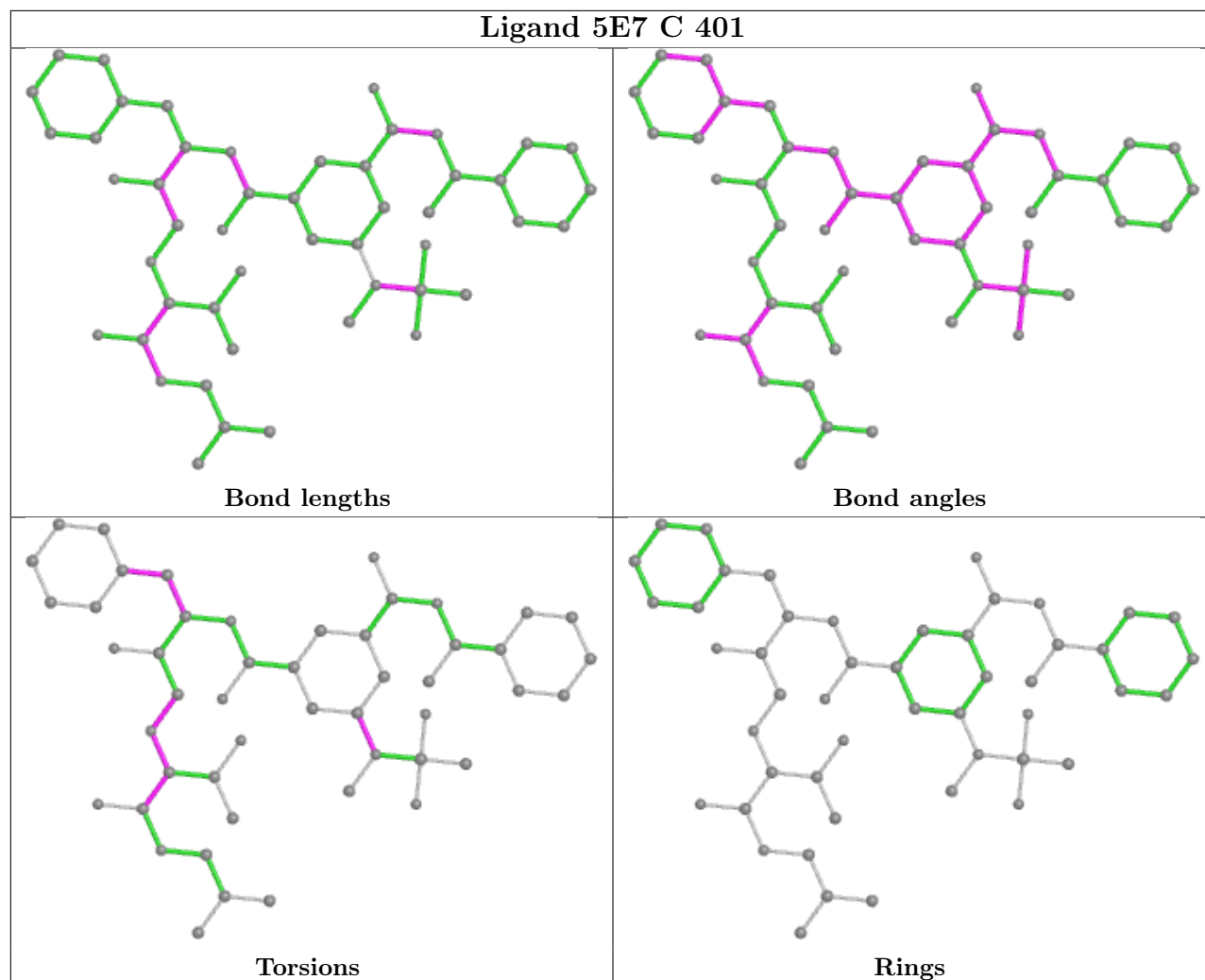
Bond angles



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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	372/390 (95%)	0.46	24 (6%)	18 15	39, 57, 82, 101	12 (3%)
1	B	369/390 (94%)	0.74	54 (14%)	2 1	38, 62, 100, 115	25 (6%)
1	C	373/390 (95%)	0.49	29 (7%)	13 9	40, 56, 78, 111	15 (4%)
All	All	1114/1170 (95%)	0.56	107 (9%)	8 5	38, 58, 89, 115	52 (4%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	272	ALA	7.1
1	B	386	ILE	5.7
1	B	257	PHE	5.6
1	C	257	PHE	5.4
1	B	273	GLY	5.3
1	B	274	THR	5.2
1	B	319	CYS	4.6
1	B	268	VAL	4.6
1	C	365	PHE	4.5
1	B	270	TRP	4.5
1	B	23	PRO	4.1
1	B	57	SER	3.9
1	A	257	PHE	3.8
1	B	365	PHE	3.8
1	C	84	LEU	3.7
1	B	271	GLN	3.7
1	B	254	THR	3.6
1	A	266	GLN	3.6
1	B	280	PHE	3.5
1	B	385	ASN	3.5
1	B	320	TYR	3.5
1	C	-3	GLY	3.5
1	B	262	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	311	ASP	3.5
1	B	44	PRO	3.5
1	C	85	VAL	3.4
1	C	197	TRP	3.4
1	B	63	LEU	3.4
1	A	42	ALA	3.4
1	A	256	LYS	3.3
1	B	269	CYS	3.3
1	B	60	TYR	3.3
1	C	61	ARG	3.2
1	C	256	LYS	3.2
1	B	277	TRP	3.2
1	A	268	VAL	3.2
1	A	-2	SER	3.2
1	B	245	VAL	3.2
1	B	275	THR	3.1
1	B	384	TYR	3.1
1	C	270	TRP	3.1
1	C	51	TYR	3.0
1	A	55	GLN	3.0
1	A	61	ARG	3.0
1	C	272	ALA	3.0
1	C	54	ARG	2.9
1	B	276	PRO	2.9
1	B	256	LYS	2.9
1	B	260	GLY	2.9
1	B	267	LEU	2.9
1	C	145	HIS	2.9
1	C	57	SER	2.8
1	C	94	THR	2.8
1	B	255	GLU	2.8
1	B	309	VAL	2.7
1	C	310	GLU	2.7
1	B	58	SER	2.7
1	C	95	VAL	2.7
1	B	362	HIS	2.7
1	B	84	LEU	2.6
1	A	60	TYR	2.6
1	B	93	VAL	2.5
1	B	56	LEU	2.5
1	B	361	VAL	2.5
1	C	268	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	261	PHE	2.5
1	B	95	VAL	2.5
1	B	363	ASP	2.5
1	B	55	GLN	2.5
1	A	279	ILE	2.5
1	A	260	GLY	2.4
1	B	22	SER	2.4
1	B	318	ASP	2.4
1	B	252	SER	2.4
1	A	365	PHE	2.3
1	B	82	THR	2.3
1	A	269	CYS	2.3
1	C	261	PHE	2.3
1	C	20	VAL	2.3
1	B	-2	SER	2.3
1	A	361	VAL	2.3
1	A	93	VAL	2.3
1	C	93	VAL	2.3
1	C	55	GLN	2.3
1	B	94	THR	2.3
1	A	56	LEU	2.3
1	A	48	LEU	2.2
1	A	270	TRP	2.2
1	A	25	GLN	2.2
1	B	197	TRP	2.2
1	C	52	TYR	2.2
1	A	20	VAL	2.2
1	C	-2	SER	2.2
1	B	59	THR	2.2
1	C	144	THR	2.2
1	A	197	TRP	2.2
1	C	21	GLY	2.1
1	B	246	LYS	2.1
1	B	306	LEU	2.1
1	A	23	PRO	2.1
1	B	253	SER	2.1
1	A	46	PRO	2.1
1	A	145	HIS	2.1
1	B	64	ARG	2.1
1	B	266	GLN	2.0
1	C	309	VAL	2.0
1	C	320	TYR	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 monosaccharides 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, 95<sup>th</sup> 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.

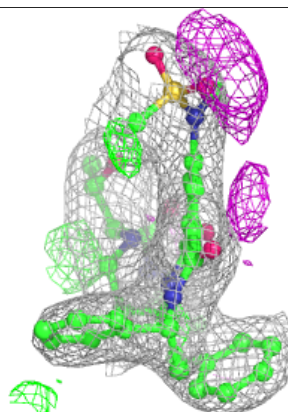
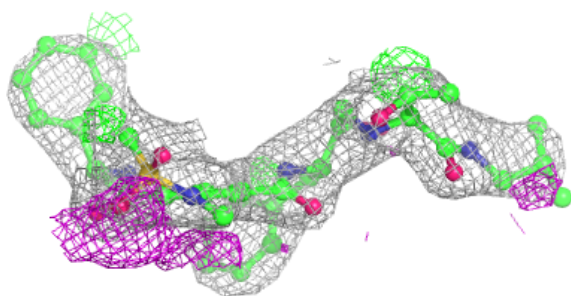
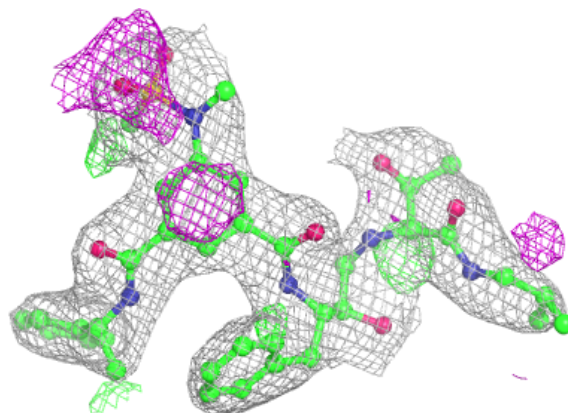
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	5E7	B	401	49/49	0.94	0.22	46,54,63,66	0
2	5E7	A	401	49/49	0.97	0.21	40,50,58,66	0
2	5E7	C	401	49/49	0.97	0.21	36,45,52,54	0

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.

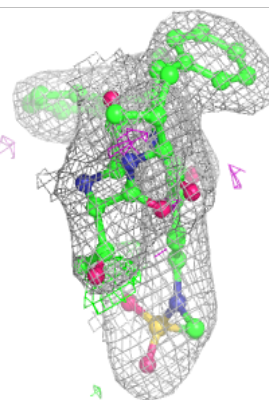
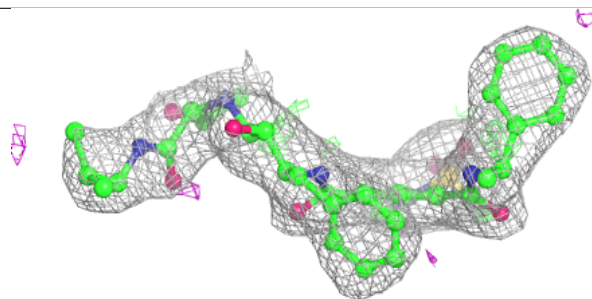
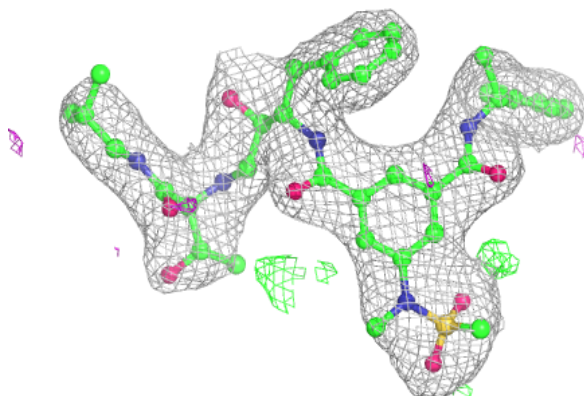


**Electron density around 5E7 B 401:**

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

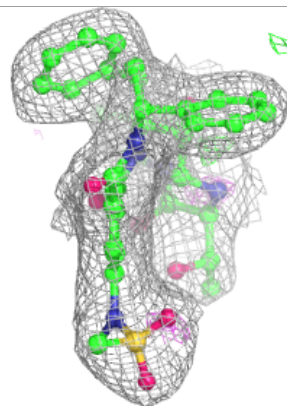
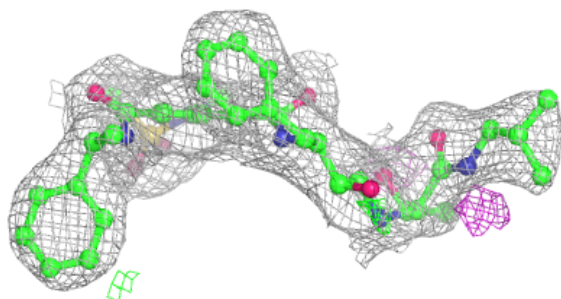
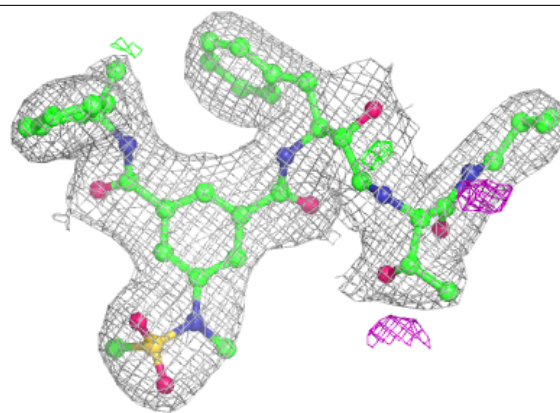
**Electron density around 5E7 A 401:**

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



**Electron density around 5E7 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 [i](#)

There are no such residues in this entry.