



Full wwPDB X-ray Structure Validation Report i

May 16, 2020 – 07:09 am BST

PDB ID : 3DM6
Title : Beta-secretase 1 complexed with statine-based inhibitor
Authors : Lindberg, J.; Borkakoti, N.; Nystrom, S.
Deposited on : 2008-06-30
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 i symbol.

The following versions of software and data (see [references](#) ①) 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	:	2.11
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)	:	2.11

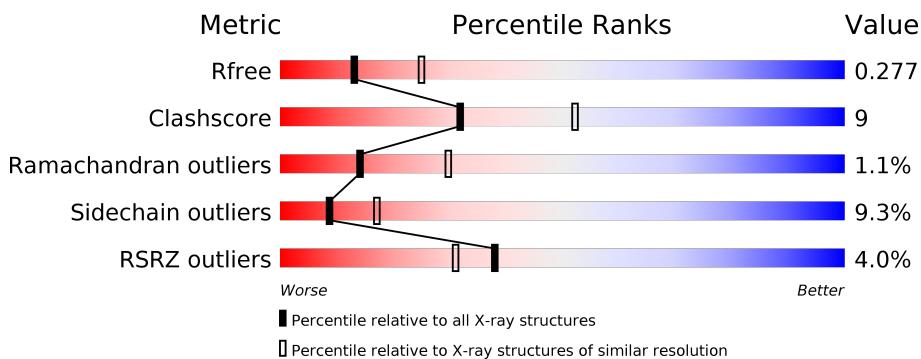
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

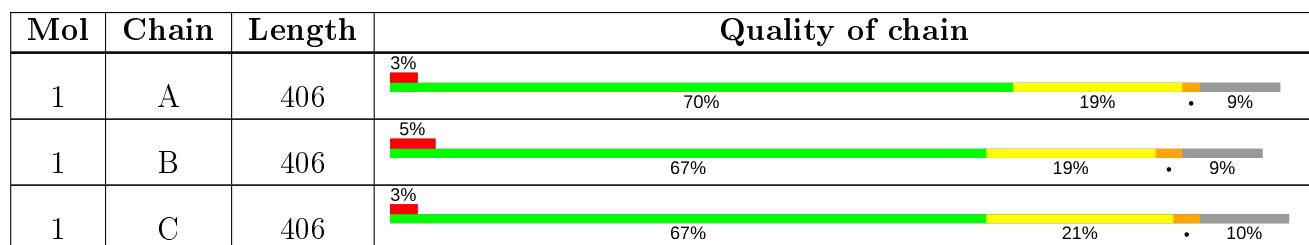
The reported resolution of this entry is 2.60 Å.

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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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%. 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.



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	757	A	1000	X	-	-	-
2	757	B	1000	X	-	-	-
2	757	C	1000	X	-	-	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8934 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.

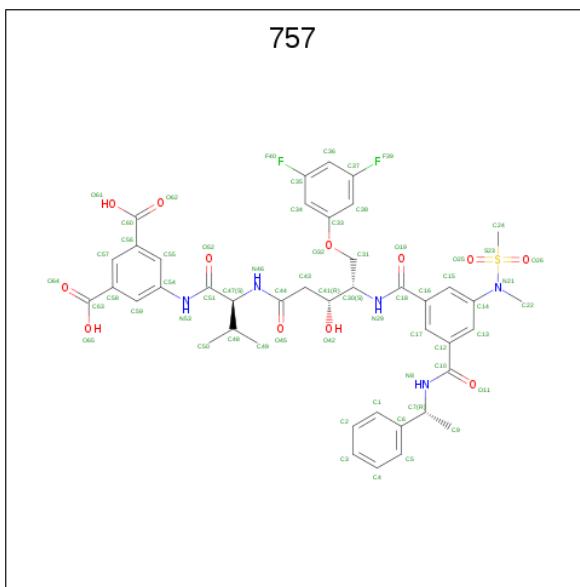
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2909	1865	485	546	13			
1	B	368	Total	C	N	O	S	0	0	0
			2902	1860	484	545	13			
1	C	367	Total	C	N	O	S	0	0	0
			2893	1855	483	542	13			

There are 3 discrepancies between the modelled and reference sequences:

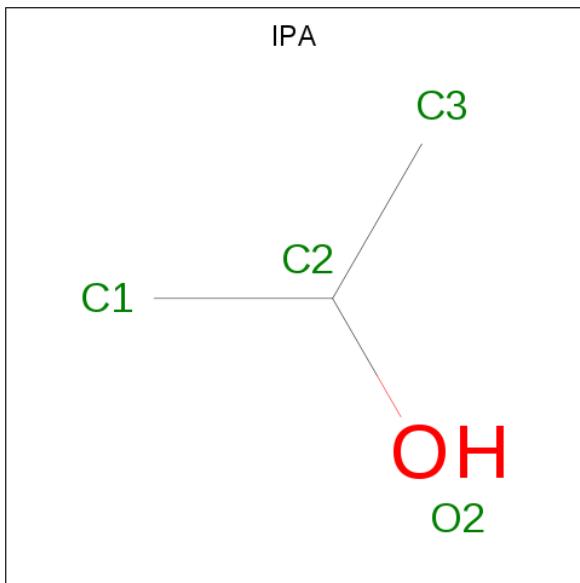
Chain	Residue	Modelled	Actual	Comment	Reference
A	28P	MET	-	INITIATING METHIONINE	UNP P56817
B	28P	MET	-	INITIATING METHIONINE	UNP P56817
C	28P	MET	-	INITIATING METHIONINE	UNP P56817

- Molecule 2 is 5-[(2S)-2-[(3R,4S)-5-(3,5-difluorophenoxy)-3-hydroxy-4-[[3-(methyl-methylsulfonyl-amino)-5-[(1R)-1-phenylethyl]carbamoyl]phenyl]carbonylamino]pentanoyl]amino]-3-methyl-butanoyl]amino]benzene-1,3-dicarboxylic acid (three-letter code: 757) (formula: C₄₂H₄₅F₂N₅O₁₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
2	A	1	62	42	2	5	12	1	0	0
2	B	1	62	42	2	5	12	1	0	0
2	C	1	62	42	2	5	12	1	0	0

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	3	1	0	0

Continued on next page...

Continued from previous page...

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

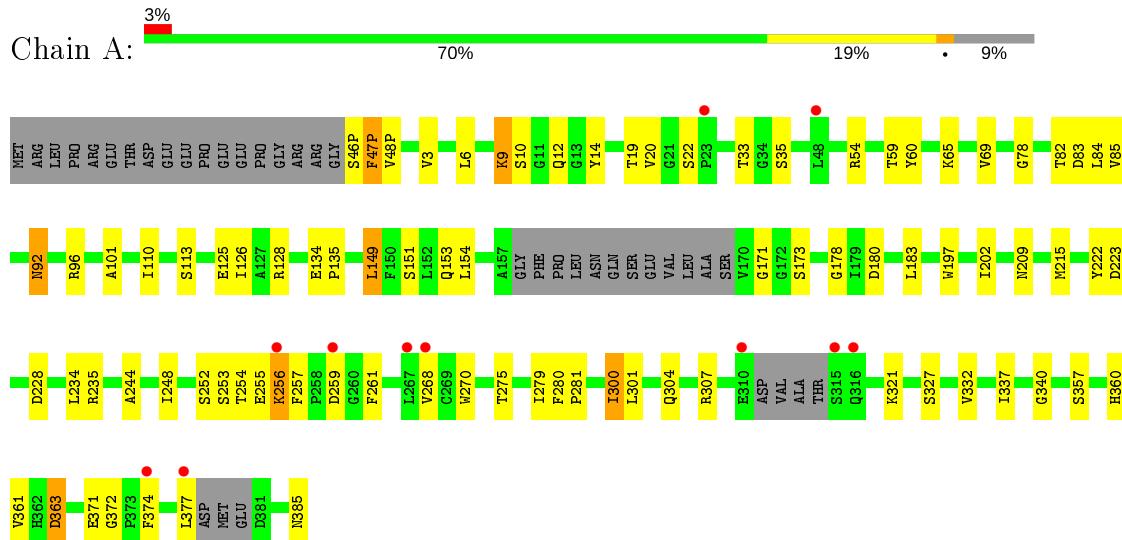
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	12	Total O 12 12	0	0
4	C	9	Total O 9 9	0	0

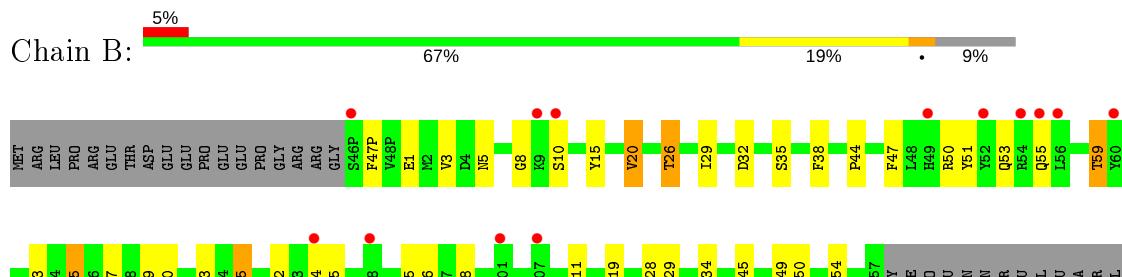
3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA and DNA 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.

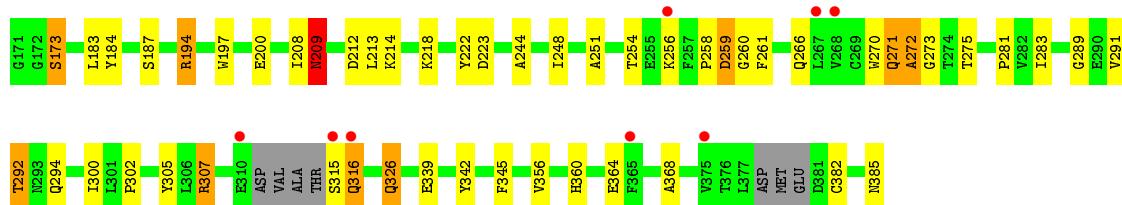
- Molecule 1: Beta-secretase 1



- Molecule 1: Beta-secretase 1

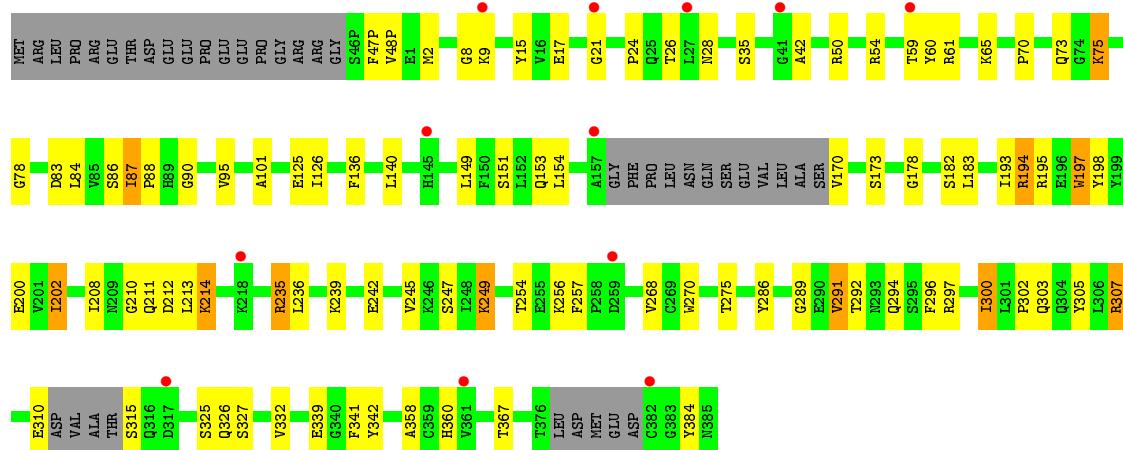


-



- Molecule 1: Beta-secretase 1





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.44Å 103.02Å 103.11Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	63.76 – 2.60 63.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (63.76-2.60) 97.6 (63.74-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ ¹	3.50 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R , R_{free}	0.223 , 0.281 0.221 , 0.277	Depositor DCC
R_{free} test set	2605 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.2	EDS
L-test for twinning ²	$< L > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8934	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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: IPA, 757

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	0.64	0/2982	0.70	0/4048
1	B	0.60	1/2975 (0.0%)	0.70	0/4038
1	C	0.60	0/2966	0.69	0/4026
All	All	0.62	1/8923 (0.0%)	0.70	0/12112

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	CYS	CB-SG	-5.02	1.73	1.81

There are no bond angle outliers.

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	2909	0	2824	49	0
1	B	2902	0	2815	52	0
1	C	2893	0	2809	54	0
2	A	62	0	43	4	0
2	B	62	0	43	2	0
2	C	62	0	43	1	0
3	A	4	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	8	0	0
3	C	4	0	8	1	0
4	A	11	0	0	0	0
4	B	12	0	0	0	0
4	C	9	0	0	0	0
All	All	8934	0	8601	155	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 9.

All (155) 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:B:26:THR:HG22	1:B:50:ARG:HH12	0.97	1.12
1:C:194:ARG:HH22	1:C:384:TYR:H	1.08	0.97
1:B:26:THR:HG22	1:B:50:ARG:NH1	1.80	0.96
1:C:291:VAL:HG22	1:C:294:GLN:HB2	1.49	0.94
1:C:26:THR:HG22	1:C:50:ARG:HH12	1.34	0.91
1:C:26:THR:HG22	1:C:50:ARG:NH1	1.89	0.87
1:C:194:ARG:HH22	1:C:384:TYR:N	1.81	0.76
1:B:307:ARG:HH11	1:B:307:ARG:HG2	1.53	0.73
1:A:301:LEU:H	1:A:304:GLN:NE2	1.86	0.73
1:A:257:PHE:HD2	1:A:268:VAL:HG11	1.55	0.71
1:A:82:THR:OG1	1:A:96:ARG:NH1	2.22	0.70
1:A:46(P):SER:O	1:A:47(P):PHE:HB2	1.91	0.69
1:B:307:ARG:CG	1:B:307:ARG:HH11	2.06	0.69
1:C:291:VAL:HG22	1:C:294:GLN:CB	2.21	0.69
1:C:194:ARG:HB3	1:C:200:GLU:HG2	1.76	0.67
1:C:235:ARG:HG3	1:C:332:VAL:HB	1.75	0.67
1:A:3:VAL:HG22	1:A:183:LEU:HD11	1.79	0.65
1:C:21:GLY:O	1:C:24:PRO:HA	1.97	0.65
1:C:291:VAL:CG2	1:C:294:GLN:HB2	2.24	0.65
1:B:272:ALA:HB2	1:B:316:GLN:O	1.99	0.63
1:B:208:ILE:HD12	1:B:213:LEU:HD11	1.80	0.63
1:B:307:ARG:NH2	1:B:339:GLU:OE2	2.32	0.63
1:B:307:ARG:NH1	1:B:307:ARG:HG2	2.12	0.63
1:B:98:ASN:ND2	1:B:134:GLU:O	2.32	0.62
1:B:47:PHE:CD2	1:B:111:ASN:HB2	2.35	0.61
1:B:26:THR:O	1:B:50:ARG:NH1	2.32	0.61
1:C:194:ARG:NH2	1:C:384:TYR:H	1.90	0.61
1:B:360:HIS:CE1	1:B:368:ALA:H	2.20	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ILE:HD13	1:A:337:ILE:CD1	2.34	0.57
1:C:26:THR:O	1:C:50:ARG:NH1	2.36	0.57
1:A:256:LYS:HZ3	1:A:256:LYS:H	1.51	0.57
1:A:253:SER:C	1:A:255:GLU:H	2.08	0.56
1:A:300:ILE:HD13	1:A:337:ILE:HD12	1.87	0.56
1:B:44:PRO:HD3	1:B:51:TYR:CZ	2.41	0.56
1:A:300:ILE:HD11	1:A:337:ILE:HG23	1.88	0.55
1:C:95:VAL:HG11	1:C:140:LEU:HA	1.89	0.55
1:C:194:ARG:HG3	1:C:202:ILE:CD1	2.37	0.55
1:C:17:GLU:HG2	1:C:88:PRO:HG2	1.87	0.55
1:A:209:ASN:ND2	1:A:281:PRO:HB3	2.21	0.55
1:B:20:VAL:HG12	1:B:85:VAL:HG22	1.88	0.55
1:B:70:PRO:HA	1:B:75:LYS:HB3	1.88	0.55
1:C:300:ILE:HD11	1:C:341:PHE:HE1	1.72	0.54
1:B:5:ASN:OD1	1:B:173:SER:HA	2.08	0.54
1:C:257:PHE:HD2	1:C:268:VAL:HG11	1.74	0.54
1:C:198:TYR:CE1	3:C:1139:IPA:H13	2.43	0.53
1:B:84:LEU:HA	1:B:95:VAL:O	2.09	0.53
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.91	0.53
1:B:258:PRO:HB2	1:B:266:GLN:HE21	1.74	0.52
1:C:358:ALA:O	1:C:360:HIS:HD2	1.92	0.52
1:A:256:LYS:NZ	1:A:256:LYS:H	2.07	0.52
1:B:32:ASP:OD2	2:B:1000:757:HG1A	2.10	0.52
1:C:208:ILE:HD12	1:C:213:LEU:HD13	1.90	0.52
1:B:291:VAL:O	1:B:294:GLN:HB3	2.10	0.51
1:B:47:PHE:CE2	1:B:111:ASN:HB2	2.45	0.51
1:B:29:ILE:CG2	1:B:119:LEU:HB2	2.41	0.51
1:A:149:LEU:HD13	1:A:178:GLY:HA2	1.93	0.51
1:C:125:GLU:OE2	1:C:195:ARG:NH2	2.43	0.51
1:B:29:ILE:HG21	1:B:119:LEU:HB2	1.93	0.50
1:B:258:PRO:HB2	1:B:266:GLN:NE2	2.27	0.49
1:C:197:TRP:CD1	1:C:197:TRP:N	2.80	0.49
1:A:340:GLY:O	1:A:357:SER:HB3	2.12	0.49
1:C:47(P):PHE:CZ	1:C:178:GLY:HA3	2.47	0.49
1:A:126:ILE:HD12	2:A:1000:757:HG1C	2.43	0.49
1:A:261:PHE:CE1	1:A:268:VAL:HG22	2.47	0.49
1:C:286:TYR:HA	1:C:296:PHE:O	2.11	0.49
1:B:289:GLY:HA3	1:B:294:GLN:O	2.13	0.49
1:A:153:GLN:NE2	1:A:183:LEU:HD22	2.27	0.48
1:C:126:ILE:HG23	1:C:197:TRP:HB2	1.95	0.48
1:A:33:THR:OG1	1:A:228:ASP:HA	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:GLY:HA3	1:C:294:GLN:O	2.13	0.48
1:A:14:TYR:CG	1:A:154:LEU:HD22	2.49	0.48
1:C:212:ASP:C	1:C:214:LYS:H	2.17	0.48
1:A:54:ARG:HD2	1:A:60:TYR:CZ	2.48	0.48
1:C:302:PRO:HA	1:C:305:TYR:CE2	2.48	0.48
1:A:270:TRP:CE3	1:A:275:THR:HG23	2.49	0.47
1:B:209:ASN:HB2	1:B:281:PRO:CB	2.44	0.47
1:C:78:GLY:HA3	1:C:101:ALA:O	2.14	0.47
1:A:20:VAL:HG12	1:A:85:VAL:HG22	1.96	0.47
1:C:194:ARG:HG3	1:C:202:ILE:HD11	1.95	0.47
1:C:307:ARG:HH12	1:C:339:GLU:CD	2.18	0.47
1:B:59:THR:HB	1:B:96:ARG:HH22	1.80	0.47
1:A:6:LEU:O	1:A:171:GLY:HA2	2.15	0.47
1:B:149:LEU:C	1:B:149:LEU:HD23	2.36	0.46
1:A:371:GLU:O	1:A:374:PHE:HE1	1.98	0.46
1:A:126:ILE:HD12	2:A:1000:757:H50A	1.99	0.45
1:A:363:ASP:OD1	1:A:363:ASP:C	2.54	0.45
1:B:69:VAL:HG22	1:B:128:ARG:HB2	1.97	0.45
1:B:150:PHE:CE2	1:B:345:PHE:CD2	3.05	0.45
1:C:193:ILE:O	1:C:194:ARG:C	2.55	0.45
1:A:257:PHE:CD2	1:A:268:VAL:HG11	2.44	0.45
1:A:92:ASN:C	1:A:92:ASN:HD22	2.20	0.45
1:A:153:GLN:HE22	1:A:183:LEU:HD22	1.81	0.45
1:B:307:ARG:HH22	1:B:339:GLU:CD	2.19	0.45
1:B:244:ALA:O	1:B:248:ILE:HG13	2.16	0.44
1:A:35:SER:CB	2:A:1000:757:H50B	2.48	0.44
1:C:54:ARG:HD2	1:C:60:TYR:CE1	2.52	0.44
1:B:302:PRO:HA	1:B:305:TYR:CE2	2.52	0.44
1:B:307:ARG:CG	1:B:307:ARG:NH1	2.71	0.44
1:A:78:GLY:HA3	1:A:101:ALA:O	2.18	0.44
1:B:8:GLY:HA2	1:B:15:TYR:CE2	2.53	0.44
1:B:271:GLN:O	1:B:273:GLY:N	2.51	0.44
1:C:235:ARG:HA	1:C:325:SER:O	2.18	0.44
1:A:180:ASP:HB3	1:A:183:LEU:HD12	1.99	0.44
1:C:194:ARG:CB	1:C:200:GLU:HG2	2.45	0.44
1:C:83:ASP:OD1	1:C:84:LEU:N	2.42	0.44
1:A:301:LEU:H	1:A:304:GLN:HE21	1.62	0.43
1:B:208:ILE:CD1	1:B:213:LEU:HD11	2.48	0.43
1:B:3:VAL:HG13	1:B:183:LEU:HD21	2.01	0.43
1:A:134:GLU:HA	1:A:135:PRO:HD3	1.66	0.43
1:C:35:SER:HA	2:C:1000:757:H50B	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:GLY:HA2	1:C:15:TYR:CE2	2.53	0.43
1:A:222:TYR:HA	1:A:223:ASP:HA	1.72	0.43
1:A:235:ARG:HG3	1:A:332:VAL:HB	2.00	0.43
1:C:136:PHE:C	1:C:136:PHE:CD2	2.91	0.43
1:C:245:VAL:O	1:C:249:LYS:HB2	2.19	0.43
1:A:372:GLY:HA2	1:A:374:PHE:CE1	2.54	0.43
1:A:280:PHE:HA	1:A:281:PRO:HD3	1.87	0.42
1:B:209:ASN:HB2	1:B:281:PRO:HB2	2.01	0.42
1:B:326:GLN:HE21	1:B:326:GLN:HB2	1.60	0.42
1:A:244:ALA:O	1:A:248:ILE:HG13	2.19	0.42
1:A:253:SER:C	1:A:255:GLU:N	2.72	0.42
1:C:210:GLY:O	1:C:211:GLN:HG2	2.19	0.42
1:B:222:TYR:HA	1:B:223:ASP:HA	1.74	0.42
1:B:67:VAL:HG23	1:B:129:PRO:HG3	2.00	0.42
1:C:197:TRP:H	1:C:197:TRP:HD1	1.67	0.42
1:A:9:LYS:O	1:A:10:SER:C	2.58	0.42
1:B:35:SER:HA	2:B:1000:757:H50B	2.01	0.42
1:B:44:PRO:HD3	1:B:51:TYR:OH	2.20	0.42
1:A:59:THR:HG21	1:A:84:LEU:HD12	2.01	0.42
1:B:59:THR:HB	1:B:96:ARG:NH2	2.34	0.42
1:C:28:ASN:HD22	1:C:28:ASN:HA	1.68	0.42
1:C:151:SER:HB2	1:C:342:TYR:CE1	2.55	0.41
1:C:270:TRP:CE3	1:C:275:THR:HG23	2.55	0.41
1:C:2:MET:CG	1:C:90:GLY:HA2	2.50	0.41
1:A:83:ASP:O	1:A:96:ARG:HA	2.20	0.41
1:B:270:TRP:CE3	1:B:275:THR:HG23	2.56	0.41
1:B:63:LEU:C	1:B:65:LYS:H	2.24	0.41
1:A:35:SER:HB2	2:A:1000:757:H50B	2.03	0.41
1:A:234:LEU:HD13	1:A:337:ILE:HD11	2.03	0.41
1:A:59:THR:HG21	1:A:84:LEU:CD1	2.50	0.41
1:B:194:ARG:NH1	1:B:200:GLU:OE2	2.54	0.41
1:B:283:ILE:HB	1:B:300:ILE:HG22	2.03	0.41
1:C:154:LEU:O	1:C:339:GLU:HA	2.21	0.41
1:C:153:GLN:OE1	1:C:183:LEU:HD22	2.21	0.41
1:C:236:LEU:O	1:C:327:SER:N	2.44	0.41
1:C:87:ILE:O	1:C:88:PRO:C	2.59	0.41
1:B:38:PHE:HE1	1:B:85:VAL:HG21	1.86	0.41
1:C:70:PRO:HA	1:C:75:LYS:HB3	2.02	0.41
1:A:110:ILE:HB	1:A:113:SER:HB3	2.03	0.41
1:A:69:VAL:HG22	1:A:128:ARG:HB2	2.02	0.41
1:A:252:SER:HA	1:A:279:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.50	0.40
1:B:154:LEU:O	1:B:339:GLU:HA	2.20	0.40
1:B:184:TYR:CD1	1:B:342:TYR:CD2	3.10	0.40
1:C:286:TYR:CE2	1:C:297:ARG:HB3	2.56	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	361/406 (89%)	333 (92%)	26 (7%)	2 (1%)	25 47
1	B	360/406 (89%)	327 (91%)	25 (7%)	8 (2%)	6 12
1	C	359/406 (88%)	325 (90%)	32 (9%)	2 (1%)	25 47
All	All	1080/1218 (89%)	985 (91%)	83 (8%)	12 (1%)	14 30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47(P)	PHE
1	B	47(P)	PHE
1	B	272	ALA
1	C	214	LYS
1	A	254	THR
1	B	209	ASN
1	B	292	THR
1	B	10	SER
1	B	251	ALA
1	B	259	ASP
1	C	303	GLN
1	B	260	GLY

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	315/347 (91%)	290 (92%)	25 (8%)	12 24
1	B	314/347 (90%)	282 (90%)	32 (10%)	7 14
1	C	313/347 (90%)	282 (90%)	31 (10%)	8 15
All	All	942/1041 (90%)	854 (91%)	88 (9%)	9 17

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48(P)	VAL
1	A	9	LYS
1	A	12	GLN
1	A	19	THR
1	A	22	SER
1	A	65	LYS
1	A	92	ASN
1	A	125	GLU
1	A	149	LEU
1	A	151	SER
1	A	173	SER
1	A	197	TRP
1	A	202	ILE
1	A	215	MET
1	A	256	LYS
1	A	259	ASP
1	A	300	ILE
1	A	307	ARG
1	A	321	LYS
1	A	327	SER
1	A	360	HIS
1	A	361	VAL
1	A	363	ASP
1	A	377	LEU
1	A	385	ASN
1	B	1	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	20	VAL
1	B	26	THR
1	B	53	GLN
1	B	55	GLN
1	B	59	THR
1	B	65	LYS
1	B	73	GLN
1	B	75	LYS
1	B	82	THR
1	B	145	HIS
1	B	173	SER
1	B	187	SER
1	B	194	ARG
1	B	197	TRP
1	B	209	ASN
1	B	212	ASP
1	B	214	LYS
1	B	218	LYS
1	B	254	THR
1	B	256	LYS
1	B	259	ASP
1	B	261	PHE
1	B	271	GLN
1	B	292	THR
1	B	307	ARG
1	B	315	SER
1	B	316	GLN
1	B	326	GLN
1	B	356	VAL
1	B	364	GLU
1	B	385	ASN
1	C	48(P)	VAL
1	C	9	LYS
1	C	59	THR
1	C	61	ARG
1	C	65	LYS
1	C	73	GLN
1	C	75	LYS
1	C	86	SER
1	C	87	ILE
1	C	149	LEU
1	C	170	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	173	SER
1	C	182	SER
1	C	194	ARG
1	C	197	TRP
1	C	202	ILE
1	C	235	ARG
1	C	239	LYS
1	C	242	GLU
1	C	247	SER
1	C	249	LYS
1	C	254	THR
1	C	256	LYS
1	C	291	VAL
1	C	292	THR
1	C	300	ILE
1	C	307	ARG
1	C	310	GLU
1	C	315	SER
1	C	326	GLN
1	C	367	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	92	ASN
1	A	114	ASN
1	A	293	ASN
1	A	304	GLN
1	A	326	GLN
1	B	28	ASN
1	B	53	GLN
1	B	55	GLN
1	B	266	GLN
1	B	271	GLN
1	B	326	GLN
1	B	360	HIS
1	B	385	ASN
1	C	28	ASN
1	C	53	GLN
1	C	73	GLN
1	C	89	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	294	GLN
1	C	360	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [\(i\)](#)

6 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	757	C	1000	-	60,65,65	1.36	5 (8%)	82,93,93	1.89	18 (21%)
2	757	A	1000	-	60,65,65	1.33	6 (10%)	82,93,93	1.98	23 (28%)
3	IPA	A	1137	-	3,3,3	0.56	0	3,3,3	0.47	0
3	IPA	B	1138	-	3,3,3	0.51	0	3,3,3	0.44	0
2	757	B	1000	-	60,65,65	1.38	5 (8%)	82,93,93	1.74	17 (20%)
3	IPA	C	1139	-	3,3,3	0.47	0	3,3,3	0.78	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	757	C	1000	-	1/1/13/17	17/59/67/67	0/4/4/4
2	757	B	1000	-	1/1/13/17	12/59/67/67	0/4/4/4
2	757	A	1000	-	1/1/13/17	12/59/67/67	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	757	C56-C60	4.91	1.52	1.47
2	C	1000	757	C56-C60	4.72	1.52	1.47
2	B	1000	757	S23-N21	-4.64	1.54	1.64
2	C	1000	757	S23-N21	-4.53	1.54	1.64
2	A	1000	757	S23-N21	-4.25	1.55	1.64
2	A	1000	757	C58-C63	4.06	1.51	1.47
2	A	1000	757	C54-N53	-3.85	1.33	1.41
2	B	1000	757	C58-C63	3.80	1.51	1.47
2	C	1000	757	C24-S23	-3.72	1.67	1.75
2	B	1000	757	C24-S23	-3.67	1.67	1.75
2	C	1000	757	C58-C63	3.63	1.51	1.47
2	A	1000	757	C24-S23	-3.58	1.67	1.75
2	B	1000	757	C54-N53	-3.47	1.34	1.41
2	C	1000	757	C54-N53	-2.49	1.36	1.41
2	A	1000	757	O26-S23	2.18	1.46	1.43
2	A	1000	757	C38-C37	2.09	1.41	1.37

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	757	O25-S23-O26	-7.61	107.73	118.59
2	A	1000	757	C43-C44-N46	6.08	124.29	116.33
2	B	1000	757	O25-S23-O26	-5.37	110.94	118.59
2	C	1000	757	C24-S23-N21	5.24	112.64	106.79
2	A	1000	757	O25-S23-O26	-4.94	111.54	118.59
2	A	1000	757	O26-S23-N21	4.83	112.89	107.08
2	A	1000	757	O32-C31-C30	4.66	116.33	108.12
2	A	1000	757	C48-C47-C51	-4.59	99.91	111.38
2	C	1000	757	O25-S23-N21	4.48	112.48	107.08
2	B	1000	757	C48-C47-C51	-3.95	101.50	111.38
2	A	1000	757	C31-O32-C33	3.91	126.21	117.93
2	B	1000	757	C43-C44-N46	3.90	121.44	116.33
2	A	1000	757	C55-C56-C60	-3.86	115.27	120.36
2	C	1000	757	O32-C31-C30	3.85	114.92	108.12
2	A	1000	757	C41-C30-N29	3.76	117.16	109.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	757	C41-C30-N29	3.65	116.95	109.92
2	C	1000	757	C48-C47-C51	-3.63	102.30	111.38
2	B	1000	757	O26-S23-N21	3.58	111.39	107.08
2	B	1000	757	O32-C31-C30	3.53	114.33	108.12
2	C	1000	757	C31-O32-C33	3.46	125.27	117.93
2	B	1000	757	C48-C47-N46	3.40	119.85	111.43
2	C	1000	757	C41-C30-N29	3.29	116.27	109.92
2	B	1000	757	O25-S23-N21	3.23	110.97	107.08
2	C	1000	757	C9-C7-C6	-3.23	104.87	112.25
2	C	1000	757	C43-C44-N46	3.20	120.53	116.33
2	A	1000	757	C57-C58-C63	3.18	124.54	120.36
2	A	1000	757	C48-C47-N46	3.16	119.25	111.43
2	B	1000	757	C59-C58-C63	-3.12	116.26	120.36
2	A	1000	757	O45-C44-N46	-3.11	117.71	122.95
2	B	1000	757	C31-O32-C33	3.07	124.43	117.93
2	C	1000	757	C16-C18-N29	3.00	122.82	117.06
2	A	1000	757	C33-C34-C35	2.91	121.46	117.56
2	B	1000	757	C33-C34-C35	2.83	121.36	117.56
2	C	1000	757	O19-C18-C16	-2.80	115.95	120.94
2	A	1000	757	C59-C58-C63	-2.65	116.87	120.36
2	C	1000	757	C33-C38-C37	2.63	121.09	117.56
2	B	1000	757	C57-C58-C63	2.61	123.79	120.36
2	B	1000	757	C36-C35-C34	-2.59	120.25	123.52
2	A	1000	757	C54-N53-C51	-2.55	121.30	127.40
2	B	1000	757	C24-S23-N21	2.53	109.61	106.79
2	C	1000	757	C33-C34-C35	2.51	120.92	117.56
2	A	1000	757	C30-N29-C18	2.47	127.51	123.01
2	C	1000	757	C48-C47-N46	2.44	117.46	111.43
2	C	1000	757	C12-C10-N8	2.42	121.70	117.06
2	A	1000	757	F39-C37-C38	2.41	121.70	118.25
2	A	1000	757	O45-C44-C43	-2.39	118.00	121.50
2	B	1000	757	O45-C44-C43	-2.38	118.01	121.50
2	A	1000	757	C33-C38-C37	2.35	120.70	117.56
2	A	1000	757	C57-C56-C55	2.26	121.66	118.31
2	B	1000	757	C57-C56-C60	2.24	123.30	120.36
2	A	1000	757	C38-C37-C36	-2.23	120.70	123.52
2	B	1000	757	C9-C7-C6	-2.12	107.41	112.25
2	A	1000	757	C38-C33-C34	-2.12	117.61	120.98
2	C	1000	757	C6-C7-N8	2.11	116.18	111.31
2	C	1000	757	C12-C13-C14	2.07	121.95	119.59
2	C	1000	757	O25-S23-C24	-2.06	105.66	108.44
2	A	1000	757	C57-C56-C60	2.06	123.07	120.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	757	O42-C41-C30	-2.01	105.80	109.85

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1000	757	C41
2	A	1000	757	C41
2	B	1000	757	C41

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1000	757	C13-C14-N21-S23
2	C	1000	757	C15-C14-N21-S23
2	C	1000	757	C14-N21-S23-O25
2	C	1000	757	N29-C30-C31-O32
2	C	1000	757	C41-C30-C31-O32
2	C	1000	757	N29-C30-C41-O42
2	C	1000	757	C31-C30-C41-C43
2	A	1000	757	C13-C14-N21-S23
2	A	1000	757	C15-C14-N21-S23
2	A	1000	757	C14-N21-S23-O25
2	A	1000	757	N29-C30-C31-O32
2	A	1000	757	C41-C30-C31-O32
2	B	1000	757	C13-C14-N21-S23
2	B	1000	757	C15-C14-N21-S23
2	B	1000	757	C14-N21-S23-O25
2	B	1000	757	N29-C30-C31-O32
2	B	1000	757	C41-C30-C31-O32
2	B	1000	757	C51-C47-C48-C50
2	A	1000	757	N46-C47-C48-C49
2	B	1000	757	N46-C47-C48-C49
2	C	1000	757	C51-C47-C48-C49
2	C	1000	757	C51-C47-C48-C50
2	B	1000	757	C51-C47-C48-C49
2	C	1000	757	N46-C47-C48-C49
2	C	1000	757	N46-C47-C48-C50
2	B	1000	757	N46-C47-C48-C50
2	A	1000	757	N46-C47-C48-C50
2	A	1000	757	C51-C47-C48-C50
2	A	1000	757	C51-C47-C48-C49
2	A	1000	757	C59-C54-N53-C51

Continued on next page...

Continued from previous page...

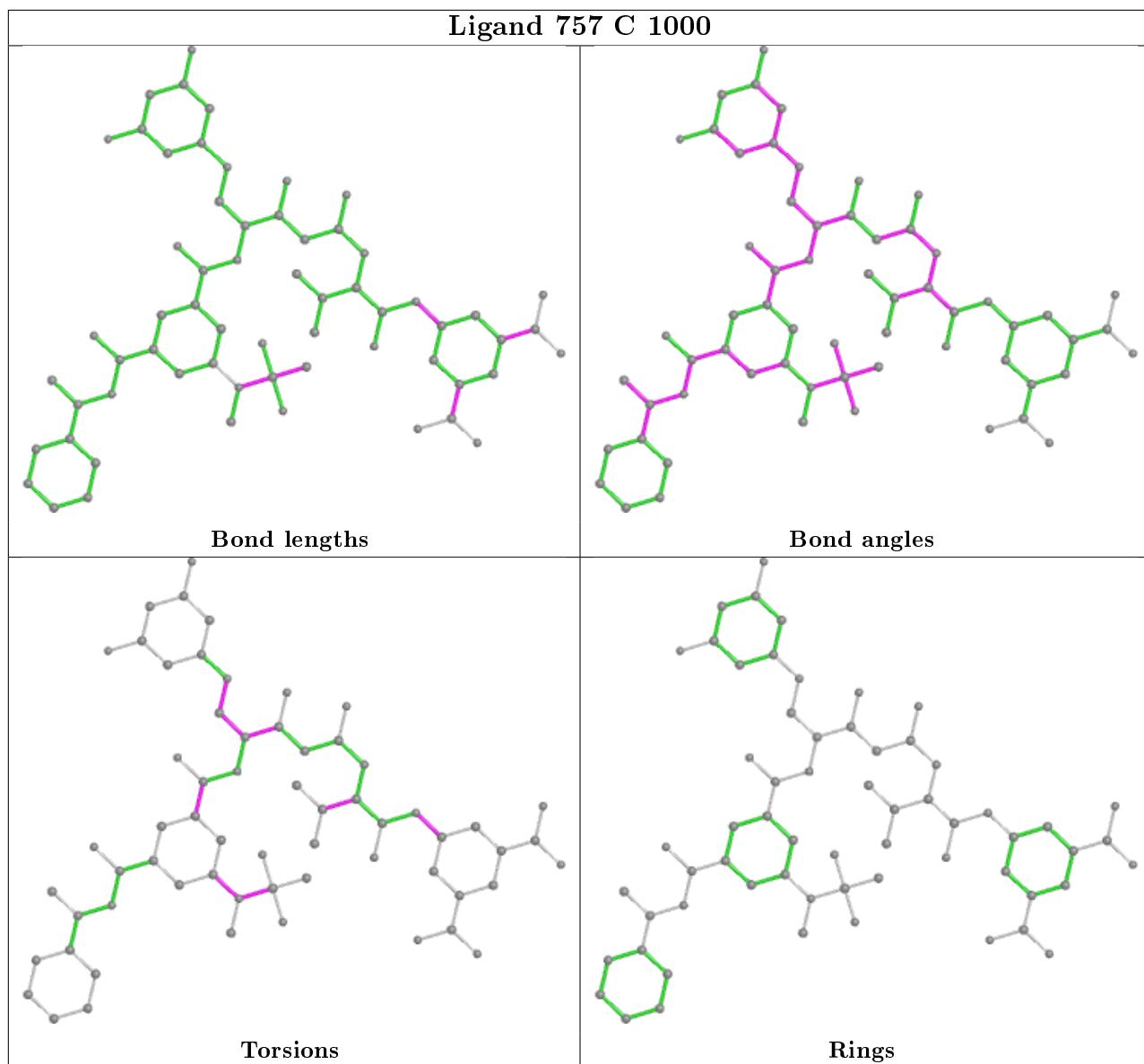
Mol	Chain	Res	Type	Atoms
2	A	1000	757	C55-C54-N53-C51
2	B	1000	757	C55-C54-N53-C51
2	B	1000	757	C59-C54-N53-C51
2	C	1000	757	C55-C54-N53-C51
2	C	1000	757	C59-C54-N53-C51
2	C	1000	757	C31-C30-C41-O42
2	C	1000	757	C17-C16-C18-O19
2	C	1000	757	C30-C31-O32-C33
2	A	1000	757	C30-C31-O32-C33
2	B	1000	757	C30-C31-O32-C33
2	C	1000	757	N29-C30-C41-C43

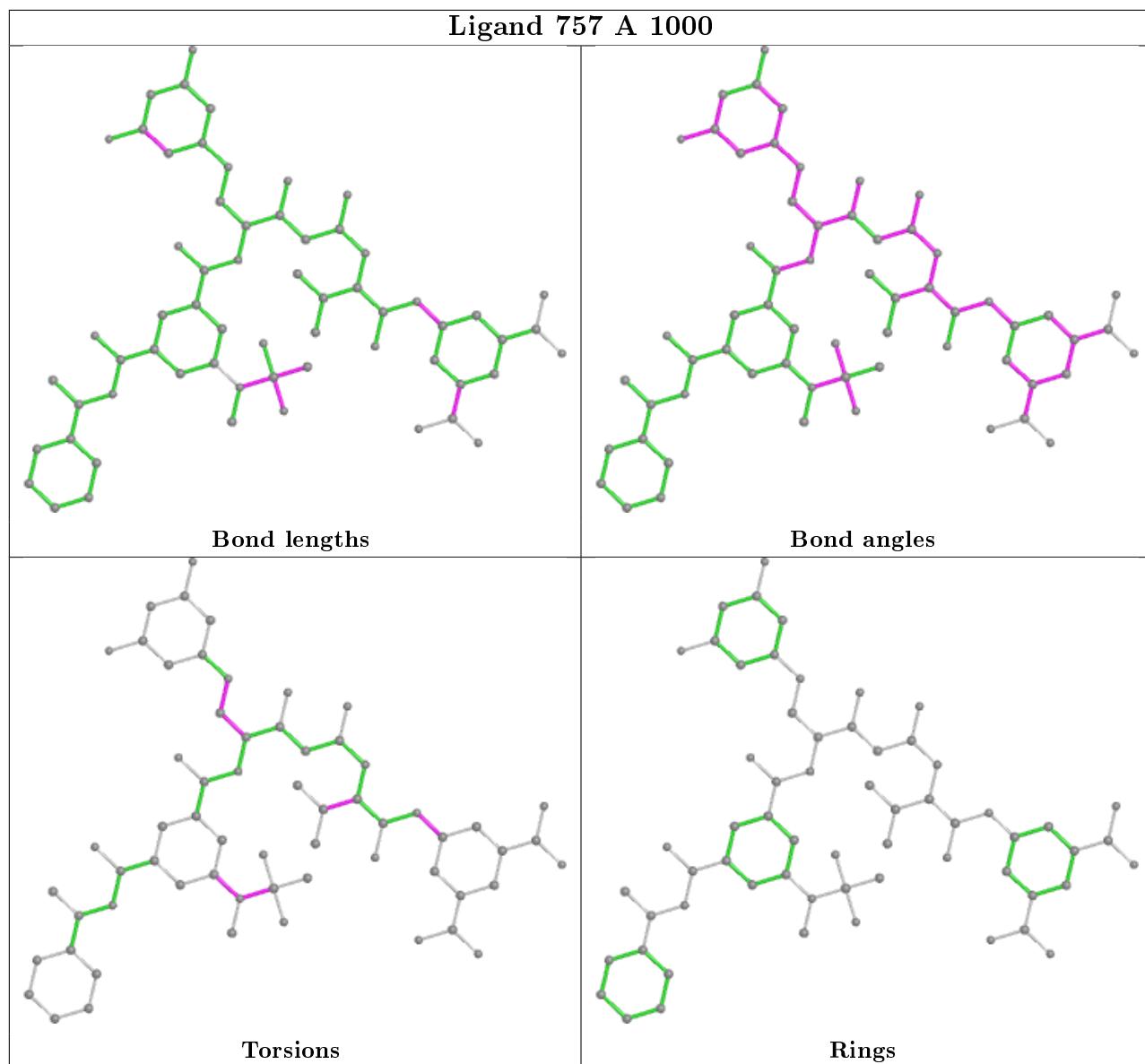
There are no ring outliers.

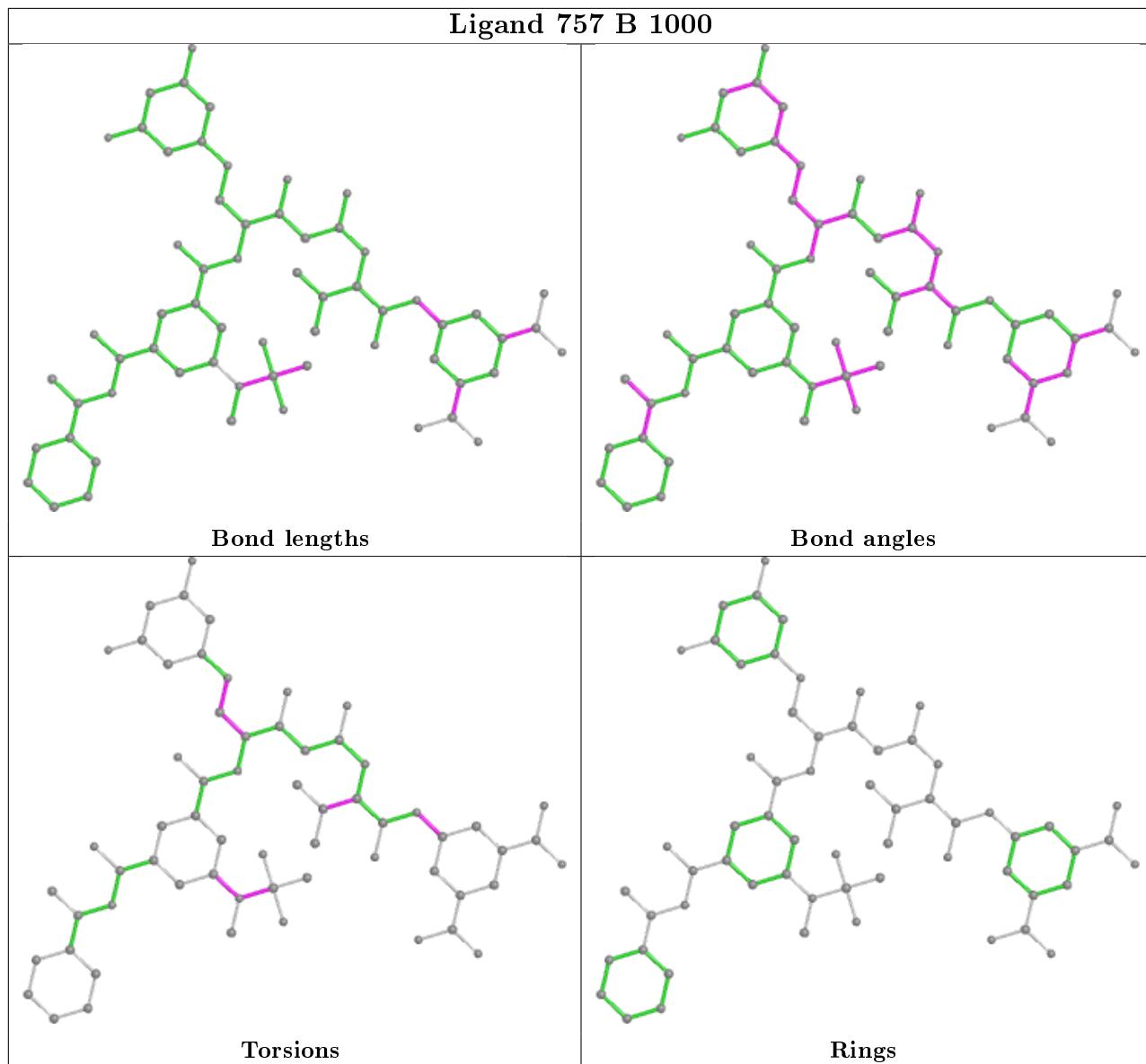
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1000	757	1	0
2	A	1000	757	4	0
2	B	1000	757	2	0
3	C	1139	IPA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	369/406 (90%)	0.57	11 (2%) 50 43	37, 60, 85, 98	3 (0%)
1	B	368/406 (90%)	0.71	21 (5%) 23 18	46, 64, 95, 105	3 (0%)
1	C	367/406 (90%)	0.56	12 (3%) 46 39	45, 66, 88, 99	3 (0%)
All	All	1104/1218 (90%)	0.61	44 (3%) 38 31	37, 64, 89, 105	9 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	LYS	6.0
1	B	10	SER	4.7
1	A	315	SER	4.0
1	B	316	GLN	3.7
1	B	49	HIS	3.5
1	B	107	LYS	3.2
1	B	268	VAL	2.9
1	A	267	LEU	2.9
1	A	316	GLN	2.7
1	B	46(P)	SER	2.7
1	A	256	LYS	2.6
1	B	101	ALA	2.6
1	B	56	LEU	2.5
1	C	21	GLY	2.5
1	A	377	LEU	2.5
1	A	259	ASP	2.4
1	B	84	LEU	2.4
1	C	145	HIS	2.3
1	B	310	GLU	2.3
1	C	59	THR	2.3
1	A	374	PHE	2.3
1	A	268	VAL	2.2
1	A	48	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	361	VAL	2.2
1	C	27	LEU	2.2
1	A	310	GLU	2.2
1	C	218	LYS	2.2
1	B	54	ARG	2.1
1	C	382	CYS	2.1
1	B	88	PRO	2.1
1	B	60	TYR	2.1
1	C	317	ASP	2.1
1	B	256	LYS	2.1
1	B	375	VAL	2.1
1	C	41	GLY	2.1
1	C	9	LYS	2.1
1	C	259	ASP	2.1
1	B	365	PHE	2.1
1	B	315	SER	2.1
1	B	267	LEU	2.1
1	A	23	PRO	2.1
1	B	55	GLN	2.0
1	C	157	ALA	2.0
1	B	52	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 carbohydrates 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.

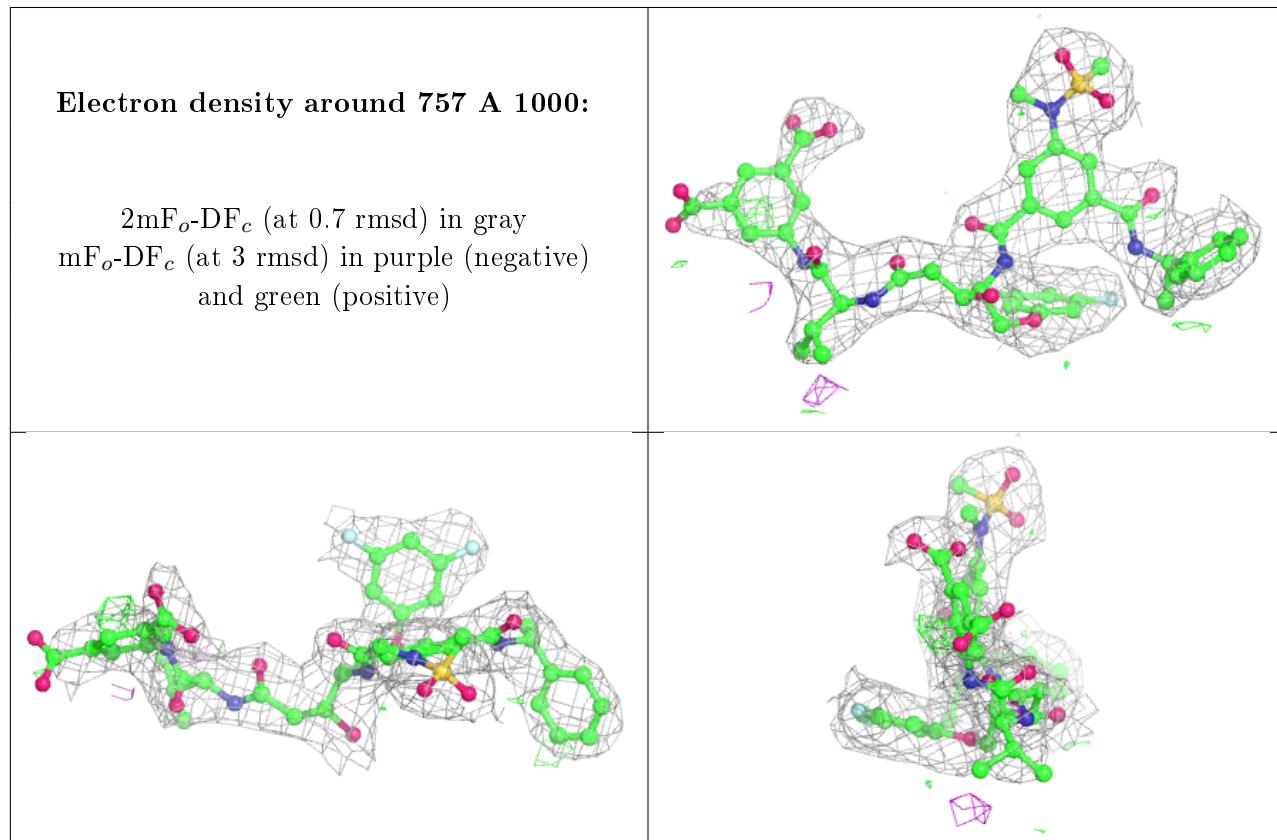
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IPA	C	1139	4/4	0.92	0.39	62,62,63,66	0
3	IPA	B	1138	4/4	0.94	0.32	54,55,56,56	0

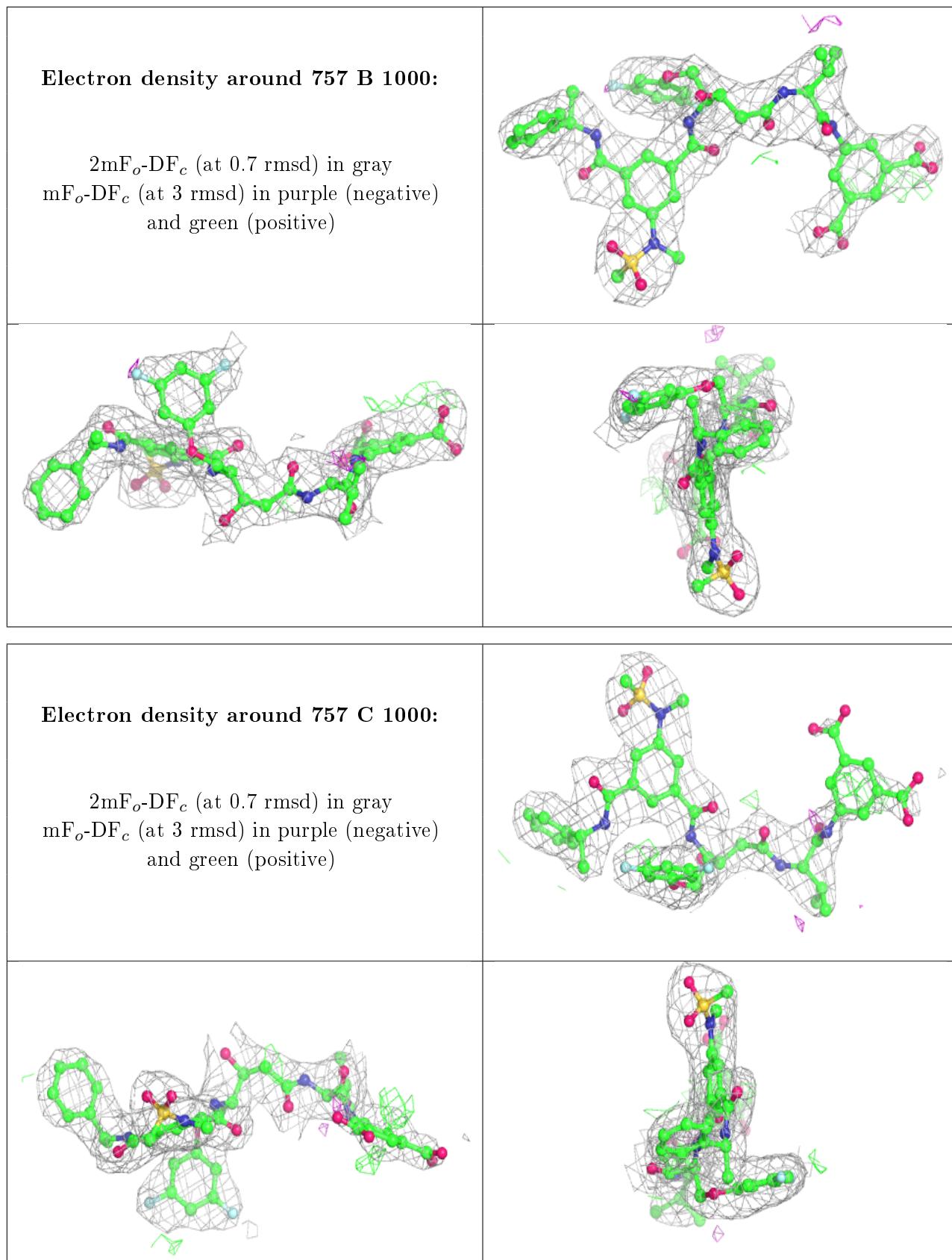
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	757	A	1000	62/62	0.94	0.27	38,54,64,65	12
2	757	B	1000	62/62	0.95	0.25	49,58,67,69	12
2	757	C	1000	62/62	0.95	0.24	38,50,60,61	12
3	IPA	A	1137	4/4	0.96	0.20	42,44,45,47	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.





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.