



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:10 PM UTC

PDB ID : 3DM6 / pdb_00003dm6
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

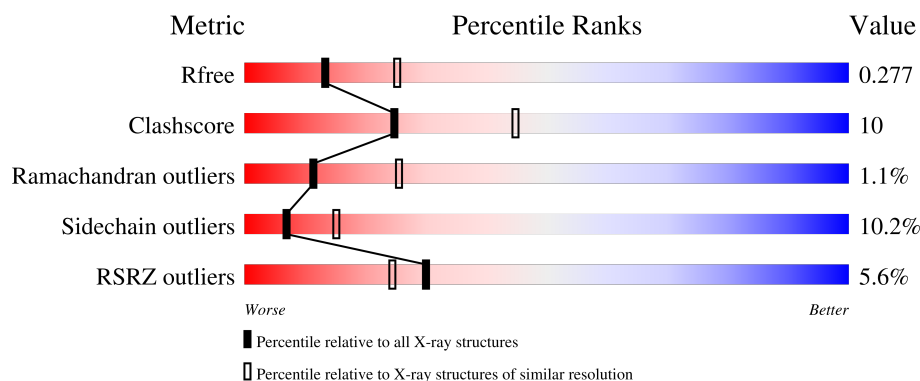
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	406	
1	B	406	
1	C	406	

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

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.

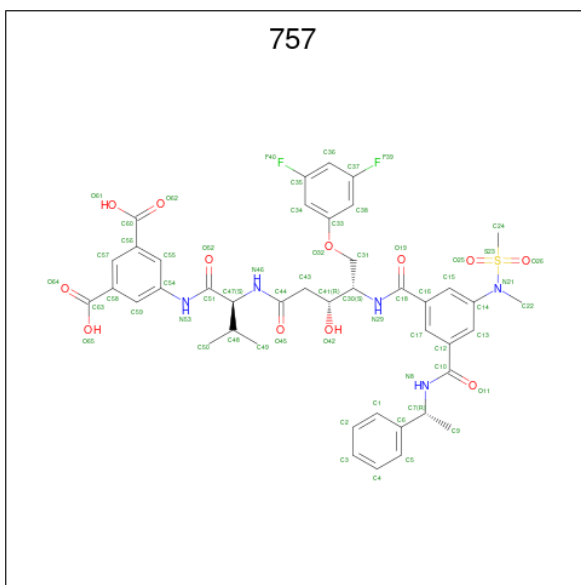
- Molecule 1 is a protein called Beta-secretase 1.

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:

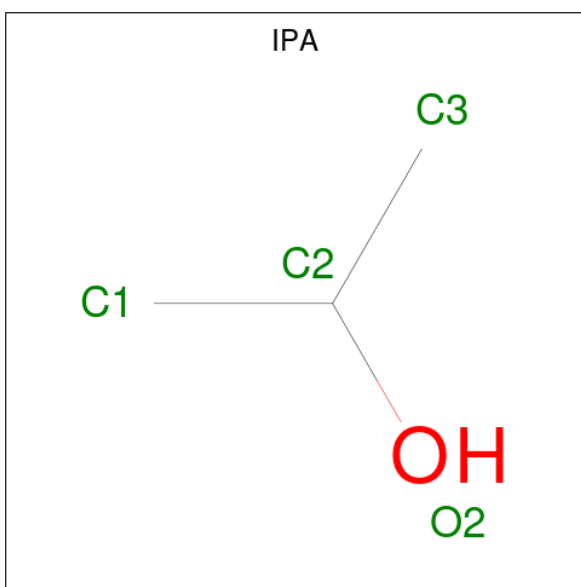
Chain	Residue	Modelled	Actual	Comment	Reference
A	28P	MET	-	initiating methionine	UNP P56817
B	28P	MET	-	initiating methionine	UNP P56817
C	28P	MET	-	initiating methionine	UNP P56817

- 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 (CCD ID: 757) (formula: C₄₂H₄₅F₂N₅O₁₂S).



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

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: $\text{C}_3\text{H}_8\text{O}$).



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

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

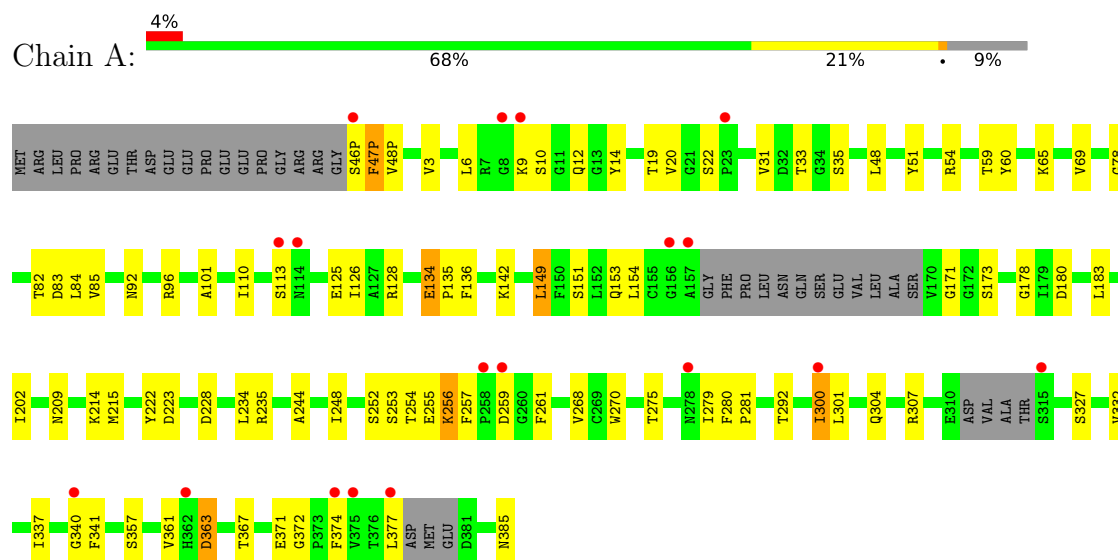
- Molecule 4 is water.

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

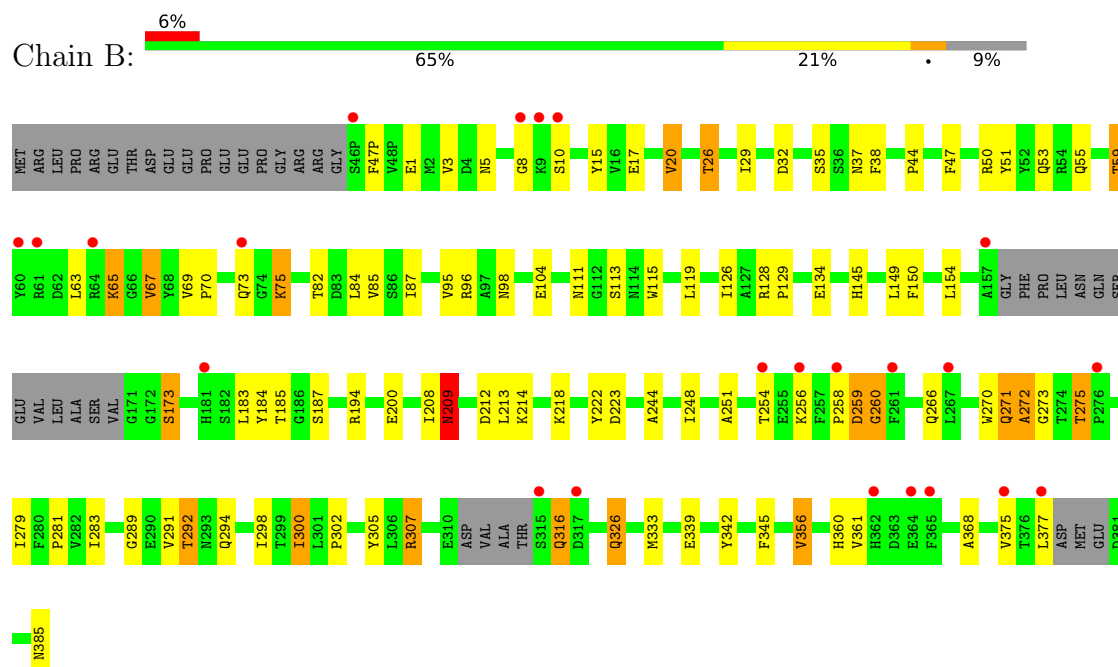
3 Residue-property plots [i](#)

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



Chain C:

40 amino acid residues are listed in a single column. Each residue is represented by a colored square (green, yellow, or red) and a red dot above it. The residues are: MET, ARG, LEU, PRO, ARG, GLU, THR, ASP, GLU, GLU, PRO, GLU, PRO, ARG, GLY, ARG, ARG, GLY, F46P, F47P, V48P, E1, M2, G8, K9, S10, Y15, V16, E17, G21, P24, Q25, T26, L27, N28, S35, G41, A42, L48, H49, R50, R54, S57, S58, T59, Y60, R61, K65, P70, Q73, G74, K75, G78, T82, D83, L84, W85, S86, I87, P88, H89, G90, T94, V95, N98, I99, A100, A101, S113, N114, W115, E125, I126, F136, L140, L149, F150, S151, L152, Q153, L154, A157, GLY, PHE, PRO, LEU, ASN, GLN, SER, VAL, LEU, ALA, SER, V170, M173, S174, I176, I177, G177, G178, S182, L183, I193, R194, R195, E196, W197, Y198, Y199, E200, V201, T202, T208, N209, G210, D211, D212, L213, M215, E219, R236, L236, K239, E242, V245, K246, S247, T248, K249, T254, F257, P258, D259, L267, V268, C269, W270, T275, N278, L285, V286, C289, E290, G290, V291, T292, N293, Q294, S295, F296, R297, I300, L301, P302, Q303, Q304, Y305, L306, R307, E310, ASP, VAL, ALA, THR, Q315, Q316, D317, S325, Q326, S327, S328, V332, M333, I337, M338, G339, G340, F341, Y342, V343, V344, A358, C359, H360, T367, P373, F374, V375, T376, LEU, ASP, MET, GLU.

4 Data and refinement statistics

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 63.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (63.76-2.60) 97.6 (63.76-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.98%)	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 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 757, IPA

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	0.77	0/2982	0.97	4/4048 (0.1%)
1	B	0.72	1/2975 (0.0%)	0.97	6/4038 (0.1%)
1	C	0.74	0/2966	0.94	2/4026 (0.0%)
All	All	0.74	1/8923 (0.0%)	0.96	12/12112 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	VAL	CA-CB	6.04	1.59	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	GLU	CA-C-N	9.40	129.16	119.76
1	A	134	GLU	C-N-CA	9.40	129.16	119.76
1	A	341	PHE	N-CA-C	6.97	120.83	110.52
1	A	51	TYR	N-CA-C	6.60	117.30	108.38
1	B	356	VAL	N-CA-CB	6.10	117.81	110.31
1	B	67	VAL	N-CA-C	5.82	116.74	108.42
1	C	198	TYR	N-CA-C	-5.82	103.03	110.53
1	B	104	GLU	N-CA-C	5.76	117.86	108.76
1	B	375	VAL	N-CA-C	5.69	116.67	108.48
1	C	328	SER	N-CA-C	-5.67	104.58	112.30
1	B	126	ILE	N-CA-C	5.53	116.83	111.91
1	B	37	ASN	N-CA-C	5.06	116.78	108.52

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	2909	0	2824	50	0
1	B	2902	0	2815	57	0
1	C	2893	0	2809	64	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
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	171	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 10.

All (171) 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:HH11	1:B:307:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ARG:HG3	1:C:332:VAL:HB	1.75	0.67
1:C:333:MET:HE2	1:C:337:ILE:HG21	1.76	0.66
1:C:174:MET:HE2	1:C:176:ILE:HD11	1.77	0.66
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:HG2	1:B:307:ARG:NH1	2.12	0.63
1:B:98:ASN:ND2	1:B:134:GLU:O	2.32	0.62
1:B:26:THR:O	1:B:50:ARG:NH1	2.32	0.61
1:B:47:PHE:CD2	1:B:111:ASN:HB2	2.35	0.61
1:A:253:SER:C	1:A:255:GLU:H	2.08	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
1:C:215:MET:HE1	1:C:239:LYS:HB3	1.84	0.59
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:H	1:A:256:LYS:HZ2	1.51	0.57
1:C:215:MET:HE2	1:C:219:GLU:HG3	1.88	0.56
1:B:298:ILE:HD11	1:B:333:MET:HE3	1.87	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:17:GLU:HG2	1:C:88:PRO:HG2	1.87	0.55
1:C:194:ARG:HG3	1:C:202:ILE:CD1	2.37	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:113:SER:HG	1:C:115:TRP:CD1	2.26	0.54
1:C:257:PHE:HD2	1:C:268:VAL:HG11	1.74	0.54
1:B:113:SER:HG	1:B:115:TRP:CD1	2.25	0.53
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:C:212:ASP:C	1:C:214:LYS:H	2.17	0.53
1:B:258:PRO:HB2	1:B:266:GLN:HE21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ALA:O	1:C:360:HIS:HD2	1.92	0.52
1:A:256:LYS:H	1:A:256:LYS:NZ	2.07	0.52
1:B:32:ASP:OD2	2:B:1000:757:H31A	2.10	0.52
1:C:208:ILE:HD12	1:C:213:LEU:HD13	1.90	0.52
1:C:307:ARG:HH12	1:C:339:GLU:CD	2.18	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:149:LEU:C	1:B:149:LEU:HD23	2.36	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:C:285:LEU:HD12	1:C:333:MET:HE3	1.94	0.50
1:A:363:ASP:OD1	1:A:363:ASP:C	2.54	0.50
1:C:193:ILE:O	1:C:194:ARG:C	2.55	0.50
1:A:92:ASN:HD22	1:A:92:ASN:C	2.20	0.49
1:B:258:PRO:HB2	1:B:266:GLN:NE2	2.27	0.49
1:B:307:ARG:HH22	1:B:339:GLU:CD	2.19	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:C50	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
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:A:54:ARG:HD2	1:A:60:TYR:CZ	2.48	0.48
1:C:136:PHE:CD2	1:C:136:PHE:C	2.91	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:C:197:TRP:CG	1:C:198:TYR:H	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:O	1:A:10:SER:C	2.58	0.46
1:B:63:LEU:C	1:B:65:LYS:H	2.24	0.46
1:A:371:GLU:O	1:A:374:PHE:HE1	1.98	0.46
1:A:253:SER:C	1:A:255:GLU:N	2.72	0.46
1:C:87:ILE:O	1:C:88:PRO:C	2.59	0.45
1:A:126:ILE:HD12	2:A:1000:757:H50A	1.99	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:A:257:PHE:CD2	1:A:268:VAL:HG11	2.44	0.45
1:A:153:GLN:HE22	1:A:183:LEU:HD22	1.81	0.45
1:C:9:LYS:O	1:C:10:SER:C	2.58	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:B:258:PRO:C	1:B:260:GLY:H	2.23	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:83:ASP:OD1	1:C:84:LEU:N	2.42	0.44
1:C:194:ARG:CB	1:C:200:GLU:HG2	2.45	0.44
1:C:213:LEU:O	1:C:214:LYS:C	2.61	0.43
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:8:GLY:HA2	1:C:15:TYR:CE2	2.53	0.43
1:C:35:SER:HA	2:C:1000:757:H50B	2.00	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: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:B:150:PHE:CD2	1:B:150:PHE:C	2.97	0.42
1:A:244:ALA:O	1:A:248:ILE:HG13	2.19	0.42
1:C:210:GLY:O	1:C:211:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:TYR:HA	1:B:223:ASP:HA	1.74	0.42
1:B:307:ARG:NH2	1:B:339:GLU:CD	2.77	0.42
1:B:67:VAL:HG23	1:B:129:PRO:HG3	2.00	0.42
1:C:197:TRP:HD1	1:C:197:TRP:H	1.67	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: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:153:GLN:OE1	1:C:183:LEU:HD22	2.21	0.41
1:C:154:LEU:O	1:C:339:GLU:HA	2.21	0.41
1:C:236:LEU:O	1:C:327:SER:N	2.44	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:69:VAL:HG22	1:A:128:ARG:HB2	2.02	0.41
1:A:110:ILE:HB	1:A:113:SER:HB3	2.03	0.41
1:A:252:SER:HA	1:A:279:ILE:HD12	2.03	0.41
1:A:135:PRO:O	1:A:136:PHE:C	2.64	0.40
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:C:302:PRO:C	1:C:304:GLN:H	2.28	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

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	361/406 (89%)	333 (92%)	26 (7%)	2 (1%)	21	42
1	B	360/406 (89%)	327 (91%)	25 (7%)	8 (2%)	5	10
1	C	359/406 (88%)	325 (90%)	32 (9%)	2 (1%)	21	42
All	All	1080/1218 (89%)	985 (91%)	83 (8%)	12 (1%)	11	25

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

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/347 (91%)	289 (92%)	26 (8%)	10	23
1	B	314/347 (90%)	280 (89%)	34 (11%)	6	13
1	C	313/347 (90%)	277 (88%)	36 (12%)	5	11
All	All	942/1041 (90%)	846 (90%)	96 (10%)	7	15

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48(P)	VAL
1	A	12	GLN
1	A	19	THR
1	A	22	SER
1	A	31	VAL
1	A	48	LEU
1	A	65	LYS
1	A	125	GLU
1	A	142	LYS
1	A	149	LEU
1	A	151	SER
1	A	173	SER
1	A	202	ILE
1	A	214	LYS
1	A	215	MET
1	A	256	LYS
1	A	259	ASP
1	A	292	THR
1	A	300	ILE
1	A	307	ARG
1	A	327	SER
1	A	361	VAL
1	A	363	ASP
1	A	367	THR
1	A	377	LEU
1	A	385	ASN
1	B	1	GLU
1	B	17	GLU
1	B	20	VAL
1	B	26	THR
1	B	53	GLN

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Mol	Chain	Res	Type
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	87	ILE
1	B	145	HIS
1	B	173	SER
1	B	185	THR
1	B	187	SER
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	271	GLN
1	B	275	THR
1	B	279	ILE
1	B	292	THR
1	B	300	ILE
1	B	307	ARG
1	B	316	GLN
1	B	326	GLN
1	B	356	VAL
1	B	377	LEU
1	B	385	ASN
1	C	48(P)	VAL
1	C	9	LYS
1	C	26	THR
1	C	48	LEU
1	C	59	THR
1	C	61	ARG
1	C	65	LYS
1	C	73	GLN
1	C	75	LYS
1	C	82	THR
1	C	86	SER
1	C	87	ILE
1	C	94	THR

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Mol	Chain	Res	Type
1	C	149	LEU
1	C	170	VAL
1	C	173	SER
1	C	182	SER
1	C	183	LEU
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	267	LEU
1	C	291	VAL
1	C	292	THR
1	C	294	GLN
1	C	300	ILE
1	C	307	ARG
1	C	310	GLU
1	C	315	SER
1	C	326	GLN
1	C	344	VAL
1	C	367	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	92	ASN
1	A	111	ASN
1	A	114	ASN
1	A	293	ASN
1	A	304	GLN
1	A	326	GLN
1	B	53	GLN
1	B	55	GLN
1	B	233	ASN
1	B	266	GLN
1	B	271	GLN
1	B	316	GLN
1	B	326	GLN
1	B	360	HIS

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Mol	Chain	Res	Type
1	C	28	ASN
1	C	53	GLN
1	C	73	GLN
1	C	89	HIS
1	C	145	HIS
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 oligosaccharides 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	$\# Z > 2$
3	IPA	C	1139	-	3,3,3	0.47	0	3,3,3	0.79	0
2	757	C	1000	-	64,65,65	1.24	3 (4%)	88,93,93	1.84	19 (21%)
2	757	A	1000	-	64,65,65	1.28	5 (7%)	88,93,93	1.91	22 (25%)
3	IPA	A	1137	-	3,3,3	0.55	0	3,3,3	0.48	0
3	IPA	B	1138	-	3,3,3	0.51	0	3,3,3	0.43	0
2	757	B	1000	-	64,65,65	1.23	3 (4%)	88,93,93	1.70	18 (20%)

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	16/67/67/67	0/4/4/4
2	757	B	1000	-	1/1/13/17	19/67/67/67	0/4/4/4
2	757	A	1000	-	1/1/13/17	19/67/67/67	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	757	S23-N21	-5.62	1.54	1.64
2	C	1000	757	S23-N21	-5.47	1.54	1.64
2	A	1000	757	S23-N21	-5.12	1.55	1.64
2	C	1000	757	C24-S23	-4.05	1.67	1.75
2	B	1000	757	C24-S23	-4.00	1.67	1.75
2	A	1000	757	C24-S23	-3.90	1.67	1.75
2	A	1000	757	C54-N53	-3.86	1.33	1.41
2	B	1000	757	C54-N53	-3.48	1.34	1.41
2	C	1000	757	C54-N53	-2.50	1.36	1.41
2	A	1000	757	O26-S23	2.15	1.46	1.43
2	A	1000	757	C38-C37	2.10	1.41	1.37

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	757	O25-S23-O26	-7.17	107.73	118.46
2	A	1000	757	C43-C44-N46	5.89	124.29	116.25
2	B	1000	757	O25-S23-O26	-5.03	110.94	118.46
2	A	1000	757	O26-S23-N21	5.03	112.89	107.14
2	A	1000	757	O32-C31-C30	4.92	116.33	108.13
2	C	1000	757	C24-S23-N21	4.76	112.64	106.82
2	A	1000	757	C48-C47-C51	-4.71	99.91	111.38
2	C	1000	757	O25-S23-N21	4.67	112.48	107.14
2	A	1000	757	O25-S23-O26	-4.62	111.54	118.46
2	C	1000	757	O32-C31-C30	4.07	114.92	108.13
2	B	1000	757	C48-C47-C51	-4.05	101.50	111.38
2	A	1000	757	C41-C30-N29	3.83	117.16	109.97
2	A	1000	757	C31-O32-C33	3.80	126.21	117.85
2	B	1000	757	C43-C44-N46	3.80	121.44	116.25
2	C	1000	757	C48-C47-C51	-3.72	102.30	111.38
2	B	1000	757	O32-C31-C30	3.72	114.33	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	757	C41-C30-N29	3.72	116.95	109.97
2	B	1000	757	O26-S23-N21	3.71	111.39	107.14
2	B	1000	757	C48-C47-N46	3.48	119.85	111.44
2	C	1000	757	C31-O32-C33	3.37	125.27	117.85
2	C	1000	757	C41-C30-N29	3.36	116.27	109.97
2	B	1000	757	O25-S23-N21	3.35	110.97	107.14
2	A	1000	757	C48-C47-N46	3.23	119.25	111.44
2	A	1000	757	C33-C34-C35	3.13	121.46	117.55
2	C	1000	757	C9-C7-C6	-3.13	104.87	112.22
2	C	1000	757	C43-C44-N46	3.13	120.53	116.25
2	C	1000	757	C16-C18-N29	3.12	122.82	117.04
2	A	1000	757	O45-C44-N46	-3.10	117.71	122.95
2	B	1000	757	C33-C34-C35	3.05	121.36	117.55
2	B	1000	757	C31-O32-C33	2.99	124.43	117.85
2	C	1000	757	C33-C38-C37	2.83	121.09	117.55
2	C	1000	757	C33-C34-C35	2.70	120.92	117.55
2	B	1000	757	C36-C35-C34	-2.68	120.25	123.50
2	A	1000	757	C54-N53-C51	-2.66	121.30	127.37
2	B	1000	757	O61-C60-C56	2.62	121.56	114.84
2	A	1000	757	C55-C56-C60	-2.62	115.27	119.96
2	A	1000	757	C57-C58-C63	2.56	124.54	119.96
2	A	1000	757	C33-C38-C37	2.53	120.70	117.55
2	C	1000	757	C12-C10-N8	2.52	121.70	117.04
2	A	1000	757	C30-N29-C18	2.51	127.51	122.94
2	C	1000	757	O19-C18-C16	-2.50	115.95	120.90
2	C	1000	757	C48-C47-N46	2.49	117.46	111.44
2	A	1000	757	O45-C44-C43	-2.42	118.00	121.54
2	B	1000	757	O45-C44-C43	-2.41	118.01	121.54
2	B	1000	757	O61-C60-O62	-2.41	118.17	123.35
2	A	1000	757	F39-C37-C38	2.41	121.70	118.28
2	A	1000	757	C38-C37-C36	-2.30	120.70	123.50
2	B	1000	757	C24-S23-N21	2.28	109.61	106.82
2	A	1000	757	O65-C63-C58	2.24	120.58	114.84
2	A	1000	757	C38-C33-C34	-2.22	117.61	120.98
2	C	1000	757	O65-C63-O64	-2.15	118.74	123.35
2	B	1000	757	C57-C58-C63	2.14	123.79	119.96
2	A	1000	757	O42-C41-C30	-2.08	105.80	109.88
2	C	1000	757	C12-C13-C14	2.07	121.95	119.61
2	B	1000	757	C59-C58-C63	-2.07	116.26	119.96
2	B	1000	757	C9-C7-C6	-2.05	107.41	112.22
2	A	1000	757	C12-C10-N8	2.04	120.83	117.04
2	C	1000	757	C6-C7-N8	2.02	116.18	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	757	O65-C63-C58	2.01	120.01	114.84

All (3) chirality outliers are listed below:

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

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	757	C13-C14-N21-S23
2	A	1000	757	C15-C14-N21-S23
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	N29-C30-C31-O32
2	B	1000	757	C41-C30-C31-O32
2	B	1000	757	C51-C47-C48-C50
2	C	1000	757	C13-C14-N21-S23
2	C	1000	757	C15-C14-N21-S23
2	C	1000	757	N29-C30-C31-O32
2	C	1000	757	C41-C30-C31-O32
2	C	1000	757	C31-C30-C41-C43
2	A	1000	757	C55-C56-C60-O61
2	B	1000	757	C57-C58-C63-O65
2	A	1000	757	C55-C56-C60-O62
2	A	1000	757	C57-C56-C60-O62
2	B	1000	757	C59-C58-C63-O64
2	B	1000	757	C57-C58-C63-O64
2	B	1000	757	C59-C58-C63-O65
2	A	1000	757	N46-C47-C48-C49
2	B	1000	757	N46-C47-C48-C49
2	A	1000	757	C57-C56-C60-O61
2	B	1000	757	C51-C47-C48-C49
2	C	1000	757	C51-C47-C48-C49
2	C	1000	757	C51-C47-C48-C50
2	A	1000	757	C57-C58-C63-O64
2	A	1000	757	C59-C58-C63-O65
2	B	1000	757	N46-C47-C48-C50

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Mol	Chain	Res	Type	Atoms
2	C	1000	757	N46-C47-C48-C49
2	C	1000	757	N46-C47-C48-C50
2	A	1000	757	C59-C58-C63-O64
2	A	1000	757	C57-C58-C63-O65
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	B	1000	757	C55-C54-N53-C51
2	A	1000	757	C59-C54-N53-C51
2	A	1000	757	C55-C54-N53-C51
2	B	1000	757	C59-C54-N53-C51
2	B	1000	757	C55-C56-C60-O62
2	B	1000	757	C57-C56-C60-O62
2	C	1000	757	C55-C54-N53-C51
2	B	1000	757	C55-C56-C60-O61
2	B	1000	757	C57-C56-C60-O61
2	C	1000	757	C59-C54-N53-C51
2	C	1000	757	C31-C30-C41-O42
2	C	1000	757	N29-C30-C41-O42
2	A	1000	757	C30-C31-O32-C33
2	B	1000	757	C30-C31-O32-C33
2	C	1000	757	C30-C31-O32-C33
2	C	1000	757	N29-C30-C41-C43
2	C	1000	757	C17-C16-C18-O19

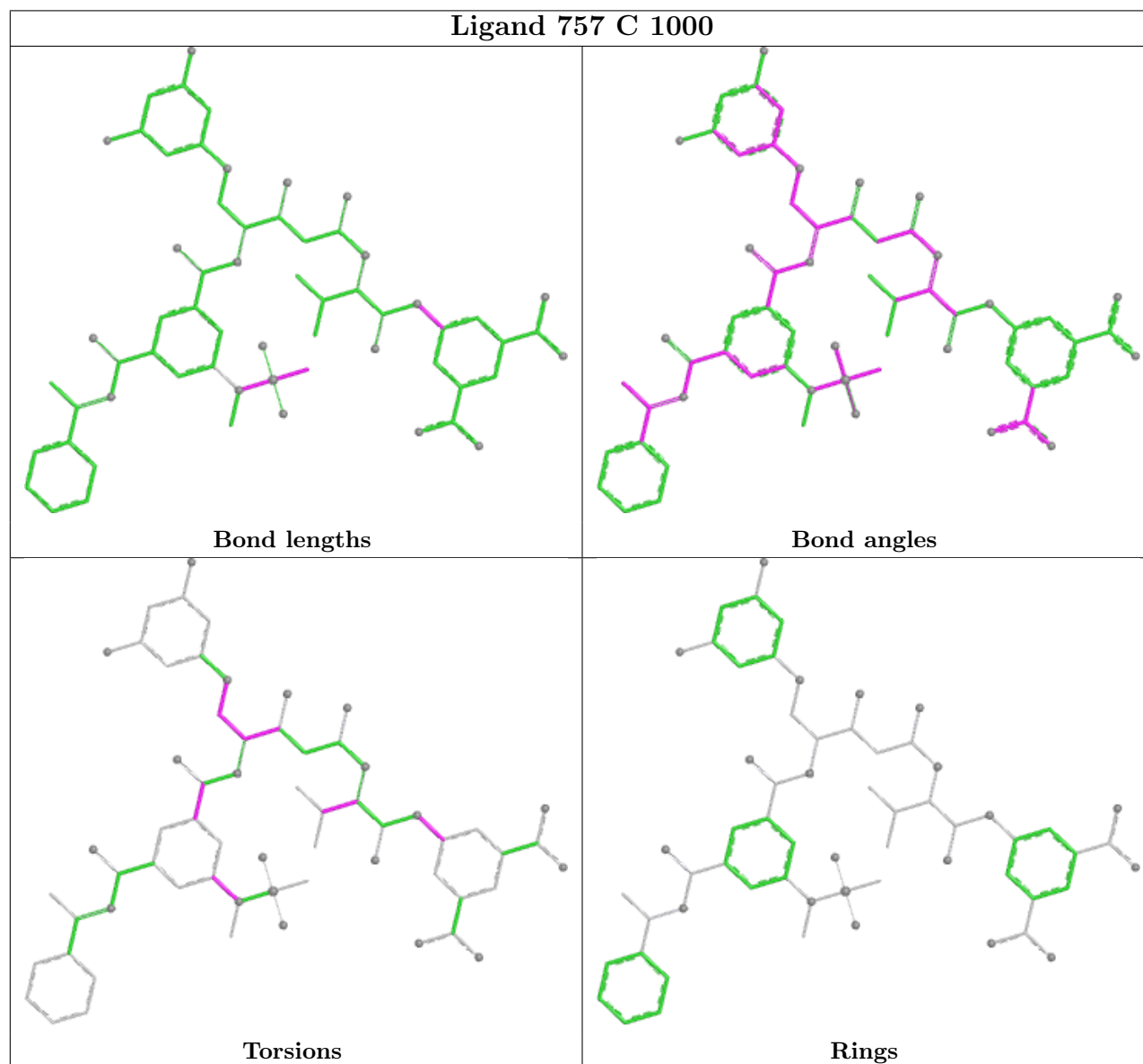
There are no ring outliers.

4 monomers are involved in 8 short contacts:

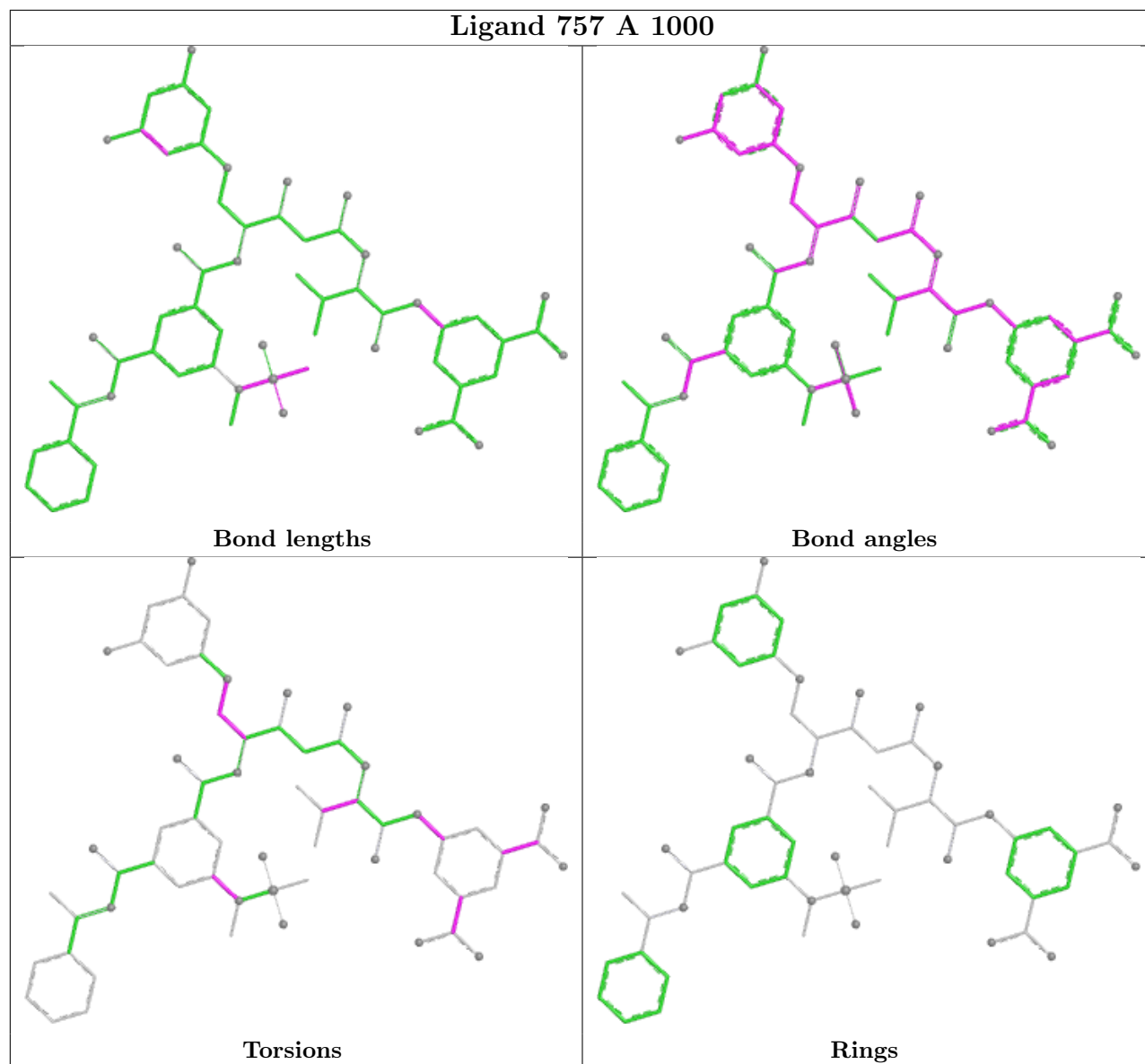
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1139	IPA	1	0
2	C	1000	757	1	0
2	A	1000	757	4	0
2	B	1000	757	2	0

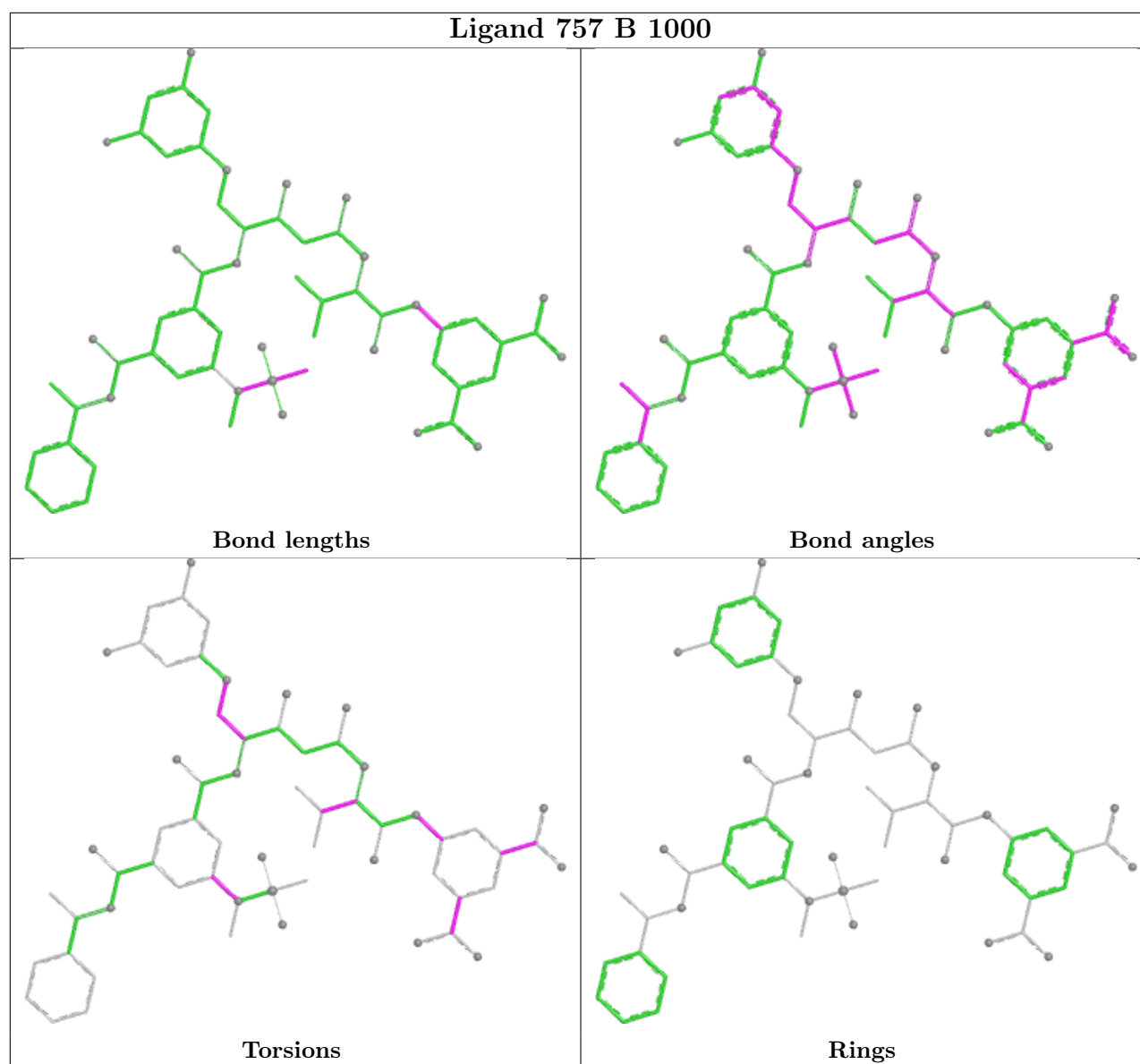
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 757 A 1000





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, 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%)	0.41	18 (4%)	35 29	37, 60, 85, 98	3 (0%)
1	B	368/406 (90%)	0.60	23 (6%)	26 20	16, 64, 95, 105	3 (0%)
1	C	367/406 (90%)	0.60	21 (5%)	29 24	38, 66, 88, 99	3 (0%)
All	All	1104/1218 (90%)	0.54	62 (5%)	30 24	16, 64, 89, 105	9 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	GLY	15.9
1	B	9	LYS	10.5
1	B	10	SER	10.0
1	A	377	LEU	7.7
1	C	9	LYS	4.2
1	B	377	LEU	4.2
1	A	258	PRO	4.1
1	C	258	PRO	3.9
1	C	8	GLY	3.5
1	A	315	SER	3.5
1	C	59	THR	3.4
1	B	362	HIS	3.2
1	A	157	ALA	3.2
1	C	21	GLY	3.2
1	A	46(P)	SER	3.1
1	C	317	ASP	3.0
1	B	157	ALA	3.0
1	A	278	ASN	2.9
1	B	256	LYS	2.9
1	C	373	PRO	2.8
1	C	259	ASP	2.8
1	C	57	SER	2.7
1	A	8	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	315	SER	2.7
1	C	382	CYS	2.6
1	A	9	LYS	2.6
1	C	316	GLN	2.6
1	A	340	GLY	2.6
1	B	258	PRO	2.6
1	B	73	GLN	2.6
1	A	375	VAL	2.5
1	A	374	PHE	2.5
1	B	254	THR	2.5
1	B	267	LEU	2.5
1	B	317	ASP	2.5
1	B	276	PRO	2.5
1	A	300	ILE	2.5
1	C	295	SER	2.5
1	C	41	GLY	2.5
1	A	113	SER	2.4
1	C	360	HIS	2.4
1	B	364	GLU	2.3
1	A	259	ASP	2.3
1	C	98	ASN	2.3
1	B	365	PHE	2.3
1	C	100	ALA	2.2
1	C	375	VAL	2.2
1	C	42	ALA	2.2
1	A	23	PRO	2.2
1	A	362	HIS	2.2
1	C	278	ASN	2.1
1	A	156	GLY	2.1
1	B	60	TYR	2.1
1	B	46(P)	SER	2.1
1	B	261	PHE	2.1
1	C	376	THR	2.1
1	C	157	ALA	2.1
1	A	114	ASN	2.1
1	B	61	ARG	2.0
1	B	64	ARG	2.0
1	B	181	HIS	2.0
1	B	375	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

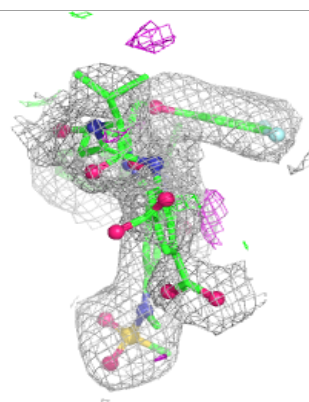
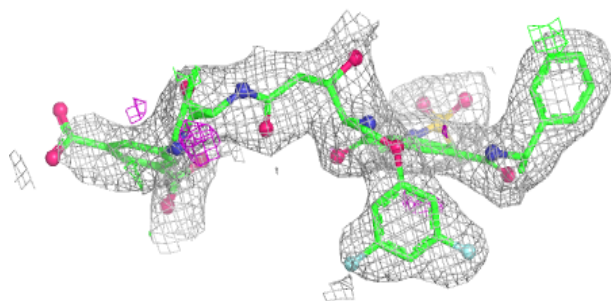
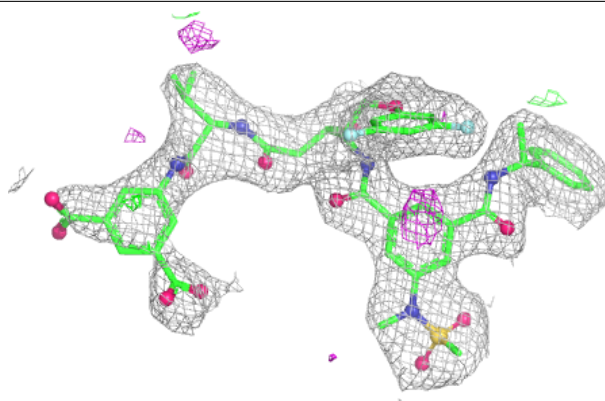
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IPA	C	1139	4/4	0.80	0.26	62,62,63,66	0
3	IPA	B	1138	4/4	0.90	0.14	54,55,56,56	0
3	IPA	A	1137	4/4	0.93	0.12	42,44,45,47	0
2	757	A	1000	62/62	0.95	0.10	38,54,64,65	12
2	757	B	1000	62/62	0.95	0.09	49,58,67,69	12
2	757	C	1000	62/62	0.95	0.11	38,50,60,61	12

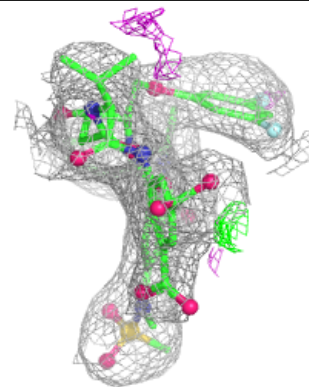
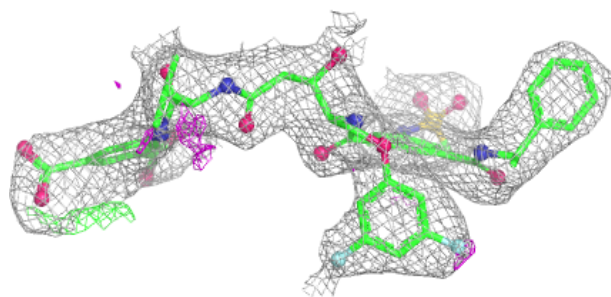
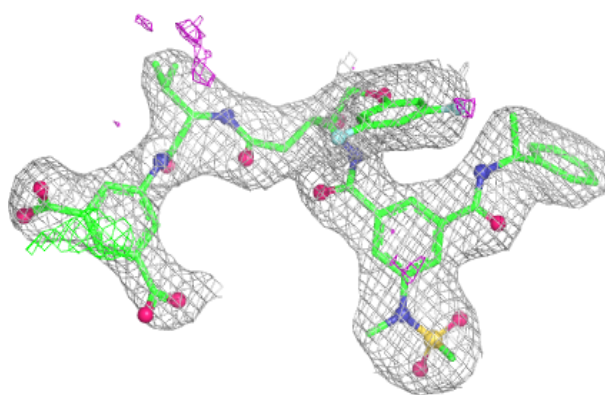
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 757 A 1000:

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

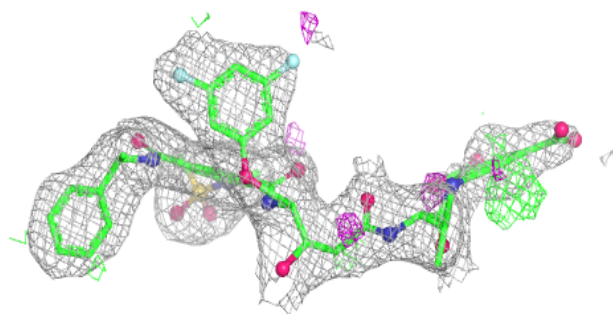
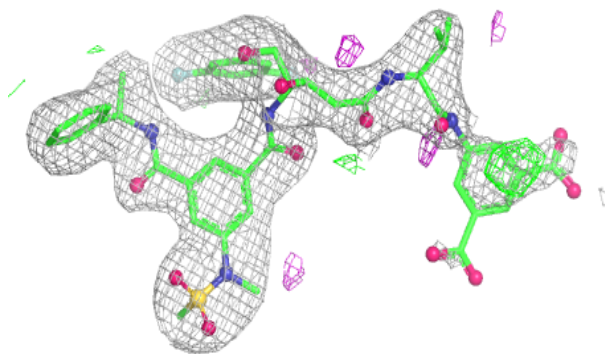
**Electron density around 757 B 1000:**

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



Electron density around 757 C 1000:

$2mF_o-DF_c$ (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.