Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 10:03 AM EDT

PDB ID	:	7UVU
Title	:	Crystal structure of human ClpP protease in complex with TR-107
Authors	:	Mabanglo, M.F.; Houry, W.A.
Deposited on	:	2022-05-02
Resolution	:	3.24 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

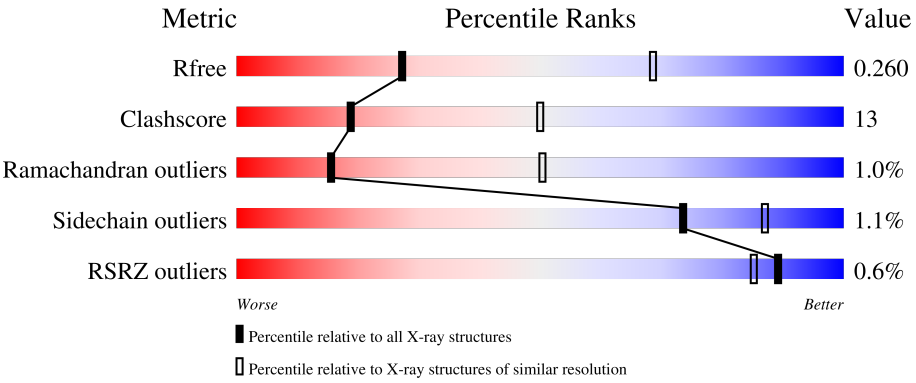
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	221	62% 16% · 20%
1	B	221	60% 20% 19%
1	C	221	50% 29% · 19%
1	D	221	59% 20% · 19%
1	E	221	62% 18% · 19%

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Mol	Chain	Length	Quality of chain
1	F	221	52% 28% 18%
1	G	221	% 56% 24% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10056 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.

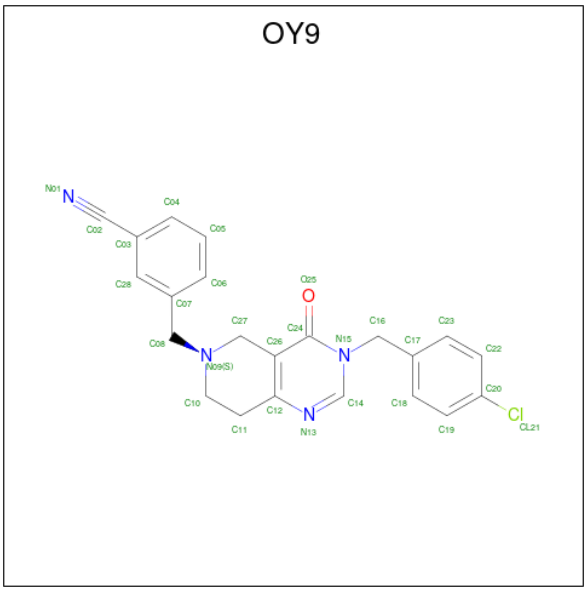
- Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1373	878	234	248	13			
1	B	178	Total	C	N	O	S	0	0	0
			1381	884	233	251	13			
1	C	178	Total	C	N	O	S	0	0	0
			1390	889	236	252	13			
1	D	179	Total	C	N	O	S	0	0	0
			1396	892	237	254	13			
1	E	179	Total	C	N	O	S	0	0	0
			1394	890	237	254	13			
1	F	181	Total	C	N	O	S	0	1	0
			1412	901	239	258	14			
1	G	178	Total	C	N	O	S	0	0	0
			1389	887	236	253	13			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	SER	-	cloning artifact	UNP Q16740
B	57	SER	-	cloning artifact	UNP Q16740
C	57	SER	-	cloning artifact	UNP Q16740
D	57	SER	-	cloning artifact	UNP Q16740
E	57	SER	-	cloning artifact	UNP Q16740
F	57	SER	-	cloning artifact	UNP Q16740
G	57	SER	-	cloning artifact	UNP Q16740

- Molecule 2 is 3-({3-[(4-chlorophenyl)methyl]-4-oxo-3,5,7,8-tetrahydropyrido[4,3-d]pyrimidin-6(4H)-yl}methyl)benzonitrile (three-letter code: OY9) (formula: $C_{22}H_{19}ClN_4O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		
2	B	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		
2	C	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		
2	D	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		
2	E	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		
2	F	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		
2	G	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	17	Total	O	0	0
			17	17		
3	C	25	Total	O	0	0
			25	25		
3	D	18	Total	O	0	0
			18	18		
3	E	17	Total	O	0	0
			17	17		

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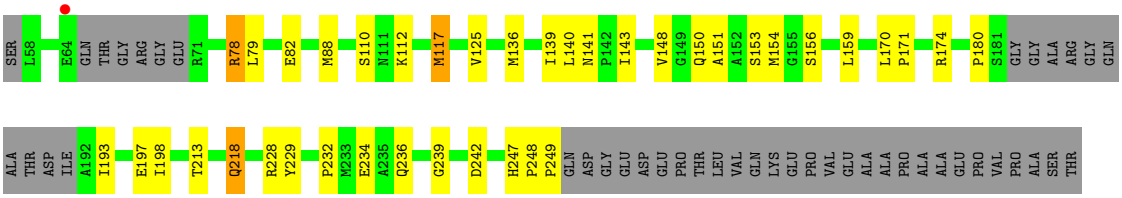
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	15	Total O 15 15	0	0
3	G	17	Total O 17 17	0	0

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.

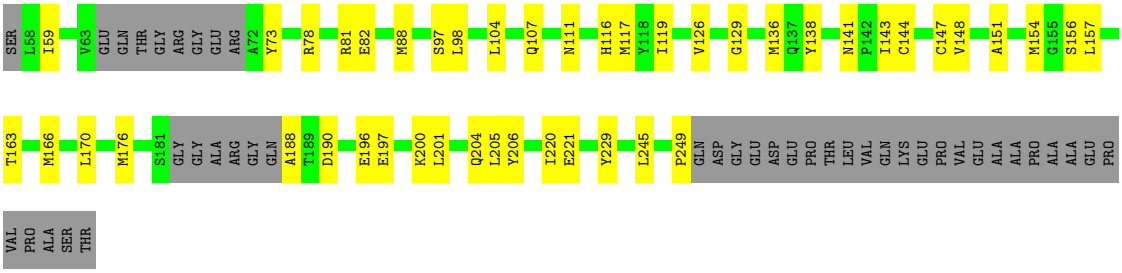
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain A:



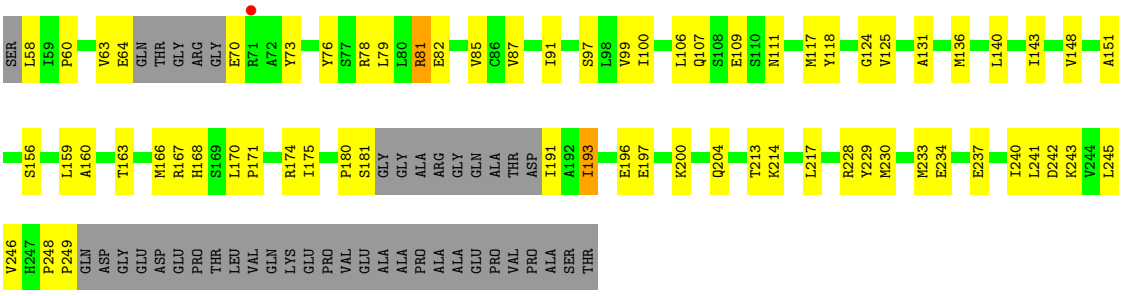
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain B:



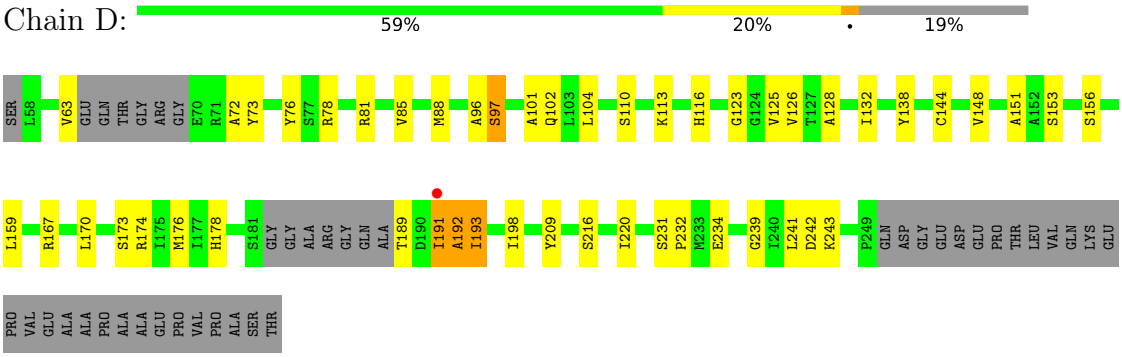
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain C:



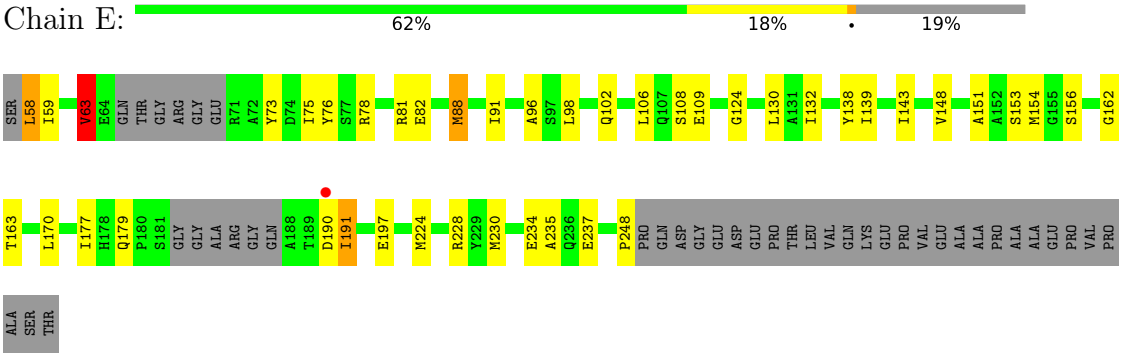
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain D:



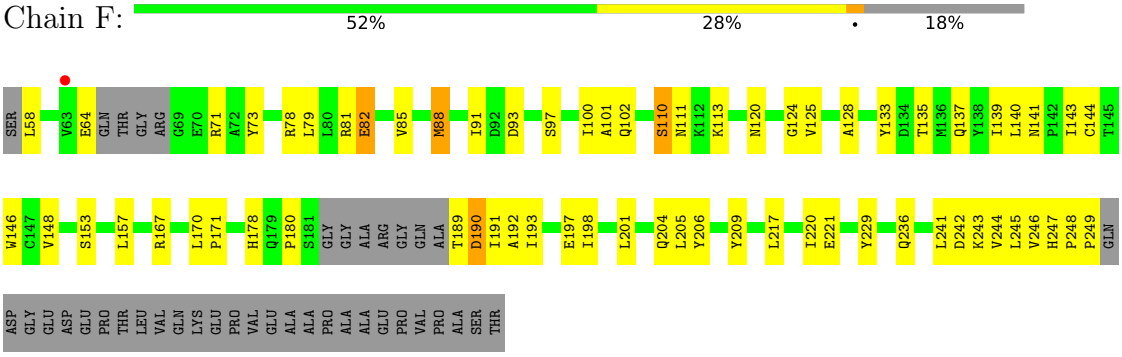
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain E:



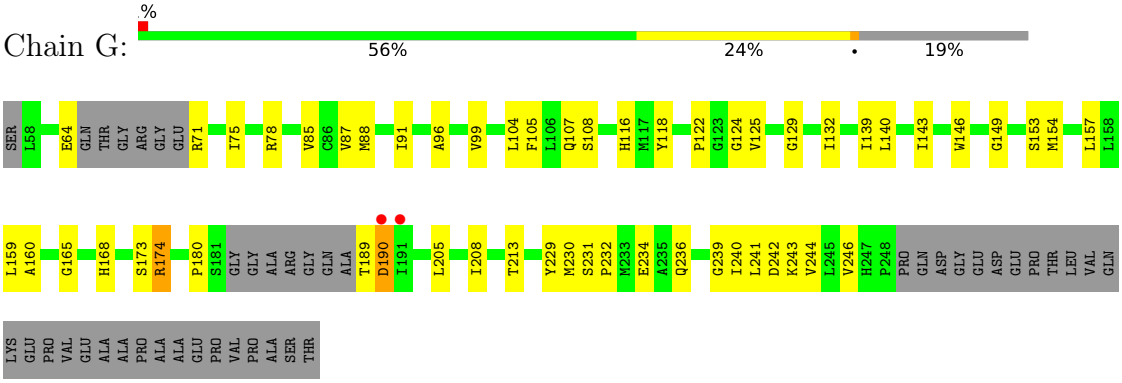
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain F:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.15Å 152.66Å 104.34Å 90.00° 118.01° 90.00°	Depositor
Resolution (Å)	48.47 – 3.24 48.47 – 3.24	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.47-3.24) 96.6 (48.47-3.24)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.190 , 0.261 0.192 , 0.260	Depositor DCC
R_{free} test set	2000 reflections (6.61%)	wwPDB-VP
Wilson B-factor (Å^2)	60.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10056	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OY9

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	0.53	0/1398	0.72	0/1891
1	B	0.54	0/1406	0.70	0/1904
1	C	0.53	0/1415	0.80	0/1914
1	D	0.55	0/1421	0.72	1/1923 (0.1%)
1	E	0.56	0/1418	0.79	3/1918 (0.2%)
1	F	0.54	0/1440	0.80	1/1948 (0.1%)
1	G	0.55	0/1413	0.78	0/1911
All	All	0.54	0/9911	0.76	5/13409 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	178	HIS	C-N-CA	-7.07	104.02	121.70
1	D	178	HIS	C-N-CA	-6.72	104.89	121.70
1	E	162	GLY	C-N-CA	-6.21	106.16	121.70
1	E	58	LEU	CA-CB-CG	-5.59	102.44	115.30
1	E	63	VAL	CB-CA-C	-5.21	101.50	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	192	ALA	Peptide

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	1373	0	1416	26	0
1	B	1381	0	1424	33	0
1	C	1390	0	1433	57	0
1	D	1396	0	1438	38	0
1	E	1394	0	1436	43	0
1	F	1412	0	1452	48	0
1	G	1389	0	1431	42	0
2	A	28	0	0	0	0
2	B	28	0	0	1	0
2	C	28	0	0	0	0
2	D	28	0	0	0	0
2	E	28	0	0	2	0
2	F	28	0	0	1	0
2	G	28	0	0	3	0
3	A	16	0	0	1	0
3	B	17	0	0	4	0
3	C	25	0	0	6	0
3	D	18	0	0	2	0
3	E	17	0	0	2	0
3	F	15	0	0	2	0
3	G	17	0	0	2	0
All	All	10056	0	10030	261	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 13.

All (261) 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)
2:G:301:OY9:C20	2:G:301:OY9:CL21	1.96	1.50
1:C:64:GLU:C	1:C:70:GLU:HB3	1.32	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:GLU:C	1:C:70:GLU:CB	2.17	1.12
1:C:64:GLU:O	1:C:70:GLU:HB3	1.51	1.09
1:C:64:GLU:O	1:C:70:GLU:CB	2.08	1.00
1:G:116:HIS:HD2	1:G:146:TRP:HE1	1.22	0.88
1:F:88:MET:HG3	1:F:120:ASN:HB3	1.55	0.86
1:G:64:GLU:HB3	1:G:71:ARG:HB3	1.58	0.84
1:B:73:TYR:OH	1:B:81:ARG:NE	2.08	0.84
1:C:70:GLU:N	3:C:401:HOH:O	2.12	0.81
1:F:73:TYR:CZ	1:F:81:ARG:HD2	2.17	0.80
1:B:78:ARG:NH2	1:B:82:GLU:OE2	2.19	0.76
1:G:230:MET:HB3	1:G:234:GLU:HB2	1.70	0.72
1:D:176:MET:HE3	3:D:408:HOH:O	1.89	0.72
1:D:123:GLY:HA3	1:D:153:SER:HB2	1.71	0.72
1:B:196:GLU:O	1:B:200:LYS:HG3	1.89	0.72
1:E:106:LEU:O	1:E:109:GLU:HB2	1.91	0.71
1:E:148:VAL:HG12	1:E:170:LEU:HD12	1.70	0.71
1:E:153:SER:OG	1:E:154:MET:N	2.24	0.70
1:G:116:HIS:HD2	1:G:146:TRP:NE1	1.90	0.69
1:C:81:ARG:NH1	3:C:402:HOH:O	2.19	0.69
1:G:105:PHE:O	1:G:108:SER:HB3	1.92	0.69
1:F:97:SER:HB2	1:G:88:MET:HG3	1.73	0.68
1:E:190:ASP:O	1:E:191:ILE:HG12	1.93	0.68
1:B:138:TYR:CE1	1:C:248:PRO:HD3	2.28	0.68
1:B:176:MET:HE3	3:B:404:HOH:O	1.94	0.68
1:A:171:PRO:O	1:A:232:PRO:HG2	1.95	0.67
1:C:107:GLN:NE2	3:C:403:HOH:O	2.20	0.66
1:B:148:VAL:HG12	1:B:170:LEU:HD12	1.77	0.66
1:F:241:LEU:O	3:F:401:HOH:O	2.13	0.66
1:B:107:GLN:HG3	1:B:141:ASN:OD1	1.95	0.65
1:C:78:ARG:HH12	1:C:82:GLU:HG2	1.62	0.65
1:G:116:HIS:CD2	1:G:146:TRP:HE1	2.11	0.63
1:D:125:VAL:HG13	1:D:189:THR:HG23	1.80	0.63
1:F:209:TYR:HB3	1:F:220:ILE:HD12	1.80	0.63
1:F:148:VAL:HG12	1:F:170:LEU:HD12	1.81	0.62
1:C:117:MET:HE3	1:C:143:ILE:HG21	1.81	0.62
1:G:236:GLN:HE21	1:G:244:VAL:HG23	1.66	0.61
1:C:171:PRO:HD3	1:C:245:LEU:O	2.01	0.61
1:C:160:ALA:HA	1:C:167:ARG:HD2	1.84	0.60
1:D:191:ILE:HG22	1:D:192:ALA:N	2.16	0.60
1:A:88:MET:HB2	3:A:415:HOH:O	2.01	0.60
1:C:233:MET:O	1:C:237:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:GLY:O	3:G:401:HOH:O	2.16	0.59
1:D:81:ARG:HH21	1:E:63:VAL:HG21	1.68	0.59
1:E:98:LEU:O	1:E:102:GLN:NE2	2.35	0.59
1:C:70:GLU:HA	1:C:70:GLU:OE1	2.02	0.58
1:C:159:LEU:HD21	1:C:241:LEU:HD21	1.85	0.58
1:F:111:ASN:HB2	1:F:140:LEU:HB2	1.84	0.58
1:F:191:ILE:O	1:F:193:ILE:HG12	2.04	0.58
1:E:139:ILE:HD11	1:E:143:ILE:HD11	1.86	0.57
1:A:153:SER:HB2	1:A:180:PRO:HD3	1.87	0.57
1:C:73:TYR:HE2	1:C:81:ARG:HD3	1.70	0.57
1:C:111:ASN:HB2	1:C:140:LEU:HD12	1.85	0.57
1:G:165:GLY:O	1:G:243:LYS:NZ	2.38	0.57
1:F:139:ILE:HD11	1:F:143:ILE:HD11	1.86	0.57
3:B:406:HOH:O	1:C:171:PRO:HG2	2.04	0.57
1:C:193:ILE:HG23	1:C:197:GLU:HB3	1.87	0.57
1:B:197:GLU:OE1	1:C:229:TYR:HB2	2.04	0.56
1:G:139:ILE:HD11	1:G:143:ILE:HD11	1.87	0.56
1:A:151:ALA:O	1:A:156:SER:HB3	2.04	0.56
1:D:138:TYR:OH	1:E:248:PRO:HB3	2.05	0.56
1:E:73:TYR:OH	1:E:81:ARG:NH1	2.38	0.56
1:C:160:ALA:HB2	1:C:240:ILE:HG23	1.89	0.55
1:A:136:MET:HG2	1:A:143:ILE:HD13	1.88	0.55
1:E:179:GLN:NE2	3:E:401:HOH:O	2.40	0.55
1:B:245:LEU:HD22	1:B:249:PRO:HD3	1.87	0.55
1:C:171:PRO:HG3	1:C:246:VAL:HG22	1.89	0.54
1:A:197:GLU:OE1	1:B:229:TYR:HB2	2.07	0.54
1:B:126:VAL:H	1:B:188:ALA:HB2	1.73	0.54
1:D:159:LEU:HD21	1:D:241:LEU:HD23	1.89	0.54
1:E:177:ILE:HG13	1:E:224:MET:HG2	1.90	0.54
1:G:168:HIS:CE1	1:G:243:LYS:HD2	2.43	0.54
1:D:138:TYR:CZ	1:E:248:PRO:HB3	2.44	0.53
1:D:192:ALA:H	1:D:193:ILE:HG23	1.73	0.53
1:B:163:THR:HB	1:B:166:MET:HE3	1.90	0.53
1:C:230:MET:HB3	1:C:234:GLU:HB2	1.90	0.52
1:D:148:VAL:HG12	1:D:170:LEU:HD12	1.89	0.52
1:B:116:HIS:ND1	1:B:144:CYS:HB2	2.23	0.52
1:A:78:ARG:NH2	1:A:82:GLU:OE1	2.42	0.52
1:E:197:GLU:CD	1:F:229:TYR:HB2	2.30	0.52
1:E:59:ILE:HD13	1:E:76:TYR:CD2	2.45	0.52
1:E:237:GLU:HG2	3:E:415:HOH:O	2.08	0.52
1:A:110:SER:O	1:A:141:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLU:HA	1:B:200:LYS:HE3	1.91	0.52
1:A:228:ARG:O	1:A:229:TYR:HB2	2.10	0.52
1:F:167:ARG:HB2	1:F:242:ASP:OD2	2.10	0.52
1:A:156:SER:HA	1:A:159:LEU:HB3	1.90	0.52
1:D:73:TYR:OH	1:D:81:ARG:NH2	2.40	0.52
1:F:73:TYR:CE2	1:F:81:ARG:HD2	2.44	0.52
1:C:78:ARG:NH1	1:C:82:GLU:HG2	2.24	0.51
1:G:236:GLN:HA	1:G:241:LEU:HB2	1.93	0.51
1:F:217:LEU:HD11	3:F:415:HOH:O	2.10	0.51
1:G:236:GLN:NE2	1:G:244:VAL:HG23	2.25	0.51
1:B:129:GLY:HA3	1:B:154:MET:HE2	1.92	0.51
1:D:81:ARG:NH2	1:E:63:VAL:HG21	2.25	0.51
1:E:96:ALA:HA	1:E:132:ILE:HD11	1.92	0.51
1:F:189:THR:HG23	1:F:190:ASP:H	1.76	0.51
1:B:197:GLU:HB2	3:B:405:HOH:O	2.11	0.50
1:E:108:SER:OG	1:E:109:GLU:N	2.44	0.50
1:E:143:ILE:H	1:E:163:THR:HG23	1.76	0.50
1:G:125:VAL:HG13	1:G:189:THR:HA	1.93	0.50
1:A:228:ARG:NH2	1:A:234:GLU:OE1	2.44	0.50
1:A:139:ILE:HD11	1:A:143:ILE:HD11	1.93	0.50
1:G:213:THR:HG22	1:G:239:GLY:O	2.11	0.50
1:A:150:GLN:NE2	1:G:190:ASP:OD2	2.45	0.49
1:D:167:ARG:NH1	1:D:239:GLY:O	2.45	0.49
1:G:174:ARG:HB3	1:G:229:TYR:CD2	2.48	0.49
1:D:101:ALA:HB1	1:E:75:ILE:HG12	1.94	0.49
1:D:126:VAL:H	1:D:189:THR:CG2	2.25	0.49
1:E:230:MET:HG2	1:E:234:GLU:HG2	1.94	0.49
1:F:110:SER:O	1:F:141:ASN:ND2	2.45	0.49
1:C:97:SER:HB2	1:D:88:MET:HG3	1.95	0.49
1:G:160:ALA:HB2	1:G:240:ILE:HG23	1.94	0.49
1:F:64:GLU:OE2	1:F:81:ARG:NH1	2.45	0.49
1:C:174:ARG:O	1:C:175:ILE:HG13	2.13	0.49
1:B:59:ILE:HD11	1:C:58:LEU:HD11	1.94	0.48
1:E:151:ALA:O	1:E:156:SER:HB3	2.13	0.48
1:D:63:VAL:HG12	1:D:72:ALA:HB2	1.95	0.48
1:A:248:PRO:HB2	1:A:249:PRO:CD	2.43	0.48
1:F:197:GLU:OE2	1:G:174:ARG:HD3	2.12	0.48
1:G:180:PRO:HB3	3:G:412:HOH:O	2.14	0.48
1:A:193:ILE:HG13	1:A:198:ILE:HG13	1.96	0.48
1:B:88:MET:HB2	3:B:416:HOH:O	2.14	0.48
1:F:110:SER:OG	1:F:113:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:MET:HG2	1:B:143:ILE:HD13	1.97	0.47
1:B:157:LEU:HD13	1:B:205:LEU:HD22	1.96	0.47
1:F:236:GLN:HE21	1:F:244:VAL:HG23	1.80	0.47
1:C:233:MET:HG2	3:C:409:HOH:O	2.15	0.47
1:D:173:SER:O	1:D:232:PRO:HD3	2.14	0.47
1:G:165:GLY:N	1:G:242:ASP:OD2	2.48	0.47
1:B:201:LEU:O	1:B:204:GLN:N	2.45	0.47
1:C:180:PRO:O	1:C:181:SER:HB2	2.15	0.47
1:D:191:ILE:HG22	1:D:192:ALA:H	1.80	0.46
1:E:197:GLU:OE1	1:F:229:TYR:HB2	2.14	0.46
1:F:71:ARG:HA	1:F:71:ARG:HD2	1.73	0.46
1:D:85:VAL:HG22	1:D:102:GLN:HB3	1.97	0.46
1:E:179:GLN:HG2	1:E:224:MET:CE	2.45	0.46
1:A:112:LYS:HE2	1:A:140:LEU:HD12	1.98	0.46
1:D:231:SER:OG	1:D:234:GLU:HG2	2.15	0.46
1:G:153:SER:OG	1:G:154:MET:N	2.47	0.46
1:A:150:GLN:HA	1:A:174:ARG:O	2.16	0.46
1:F:206:TYR:CE2	1:F:221:GLU:HG2	2.50	0.46
1:G:157:LEU:HD13	1:G:205:LEU:HD22	1.96	0.46
1:B:126:VAL:H	1:B:188:ALA:CB	2.29	0.46
1:E:228:ARG:HH12	1:E:230:MET:HG3	1.81	0.46
1:G:96:ALA:HA	1:G:132:ILE:HD11	1.98	0.46
1:E:148:VAL:CG1	1:E:170:LEU:HD12	2.43	0.46
1:E:78:ARG:NH1	1:E:82:GLU:HG2	2.31	0.46
1:G:91:ILE:HB	1:G:124:GLY:HA3	1.97	0.46
1:F:79:LEU:HA	1:F:79:LEU:HD23	1.79	0.45
1:B:104:LEU:HA	1:B:104:LEU:HD23	1.64	0.45
1:E:59:ILE:HD12	1:F:58:LEU:HD11	1.99	0.45
1:F:78:ARG:HD2	1:F:78:ARG:HA	1.70	0.45
1:A:213:THR:HA	1:A:239:GLY:O	2.16	0.45
1:D:125:VAL:HB	1:D:128:ALA:HB3	1.98	0.45
1:F:153:SER:OG	1:F:180:PRO:HD3	2.17	0.45
1:E:58:LEU:HG	1:E:59:ILE:N	2.30	0.45
1:D:116:HIS:ND1	1:D:144:CYS:HB2	2.32	0.45
1:F:133:TYR:O	1:F:137:GLN:HG2	2.17	0.45
1:A:247:HIS:HB3	1:A:248:PRO:HD2	1.98	0.45
1:B:73:TYR:HH	1:B:81:ARG:HE	1.56	0.45
1:C:64:GLU:O	1:C:70:GLU:HB2	2.06	0.45
1:C:106:LEU:O	1:C:109:GLU:HB2	2.17	0.45
1:G:78:ARG:HA	1:G:78:ARG:HD2	1.77	0.45
1:D:76:TYR:HB2	1:E:58:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:SER:OG	1:D:113:LYS:HB2	2.16	0.45
1:F:82:GLU:HG3	2:F:301:OY9:C22	2.47	0.45
1:D:96:ALA:HA	1:D:132:ILE:HD11	1.98	0.45
1:C:85:VAL:HG11	1:C:99:VAL:HG13	1.99	0.45
1:B:148:VAL:CG1	1:B:170:LEU:HD12	2.47	0.44
1:C:151:ALA:O	1:C:156:SER:HB3	2.15	0.44
1:G:64:GLU:CB	1:G:71:ARG:HB3	2.40	0.44
1:A:148:VAL:HG12	1:A:170:LEU:HB2	1.99	0.44
1:F:197:GLU:OE1	1:G:229:TYR:HB2	2.17	0.44
1:F:243:LYS:HB3	1:F:245:LEU:HD21	1.98	0.44
1:A:236:GLN:NE2	1:A:242:ASP:O	2.50	0.44
1:D:193:ILE:HD11	1:D:198:ILE:HG12	1.99	0.44
1:E:138:TYR:CE1	1:F:248:PRO:HG3	2.53	0.44
1:A:117:MET:HE2	1:A:117:MET:HB2	1.93	0.44
1:B:151:ALA:O	1:B:156:SER:HB3	2.17	0.44
1:C:200:LYS:HD2	1:D:174:ARG:NH2	2.32	0.44
1:E:191:ILE:HD11	1:F:229:TYR:OH	2.18	0.44
1:F:171:PRO:HD3	1:F:245:LEU:O	2.18	0.44
1:G:85:VAL:HG11	1:G:99:VAL:HG13	2.00	0.44
1:C:213:THR:O	1:C:214:LYS:HB2	2.18	0.43
1:E:130:LEU:HD23	1:E:130:LEU:HA	1.80	0.43
1:E:170:LEU:HD23	1:E:170:LEU:HA	1.86	0.43
1:G:157:LEU:HD21	1:G:208:ILE:HG21	1.99	0.43
1:C:100:ILE:HD11	1:C:131:ALA:HB1	1.99	0.43
1:B:98:LEU:HD11	1:C:60:PRO:HD2	2.00	0.43
1:D:81:ARG:HH21	1:E:63:VAL:CG2	2.31	0.43
1:E:234:GLU:O	1:E:237:GLU:HG3	2.19	0.43
1:F:170:LEU:HD23	1:F:245:LEU:O	2.19	0.43
1:F:193:ILE:HG22	1:F:198:ILE:HG13	2.00	0.43
1:D:242:ASP:O	1:D:243:LYS:HG3	2.19	0.43
1:E:59:ILE:HD13	1:E:76:TYR:HD2	1.83	0.43
1:G:87:VAL:HG22	1:G:99:VAL:HG21	2.00	0.43
1:G:107:GLN:OE1	1:G:140:LEU:HG	2.18	0.43
1:C:204:GLN:OE1	1:D:174:ARG:HD3	2.18	0.43
1:D:76:TYR:HB2	1:E:58:LEU:CD2	2.49	0.43
1:G:78:ARG:HG3	2:G:301:OY9:CL21	2.56	0.43
1:C:87:VAL:N	1:C:118:TYR:O	2.43	0.43
1:E:230:MET:HE2	1:E:235:ALA:HA	2.01	0.43
1:E:230:MET:CE	1:E:235:ALA:HA	2.48	0.43
1:B:206:TYR:CZ	1:B:221:GLU:HG2	2.54	0.43
1:C:64:GLU:O	1:C:70:GLU:CG	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ARG:HH22	1:C:234:GLU:CD	2.23	0.43
1:C:248:PRO:HB2	1:C:249:PRO:HD2	2.01	0.43
1:C:91:ILE:O	1:C:124:GLY:HA3	2.19	0.42
1:C:148:VAL:HG23	1:C:170:LEU:HD13	2.01	0.42
1:C:163:THR:O	1:C:166:MET:HB2	2.19	0.42
1:F:85:VAL:HG22	1:F:102:GLN:HB3	2.01	0.42
1:C:117:MET:HE1	1:C:136:MET:HG2	2.00	0.42
1:D:104:LEU:HD21	2:E:301:OY9:C05	2.49	0.42
1:F:93:ASP:OD1	1:F:128:ALA:HB2	2.19	0.42
1:F:125:VAL:HA	1:F:189:THR:HG22	2.00	0.42
1:C:228:ARG:NH2	1:C:234:GLU:OE2	2.49	0.42
1:D:151:ALA:O	1:D:156:SER:HB3	2.20	0.42
1:F:125:VAL:HB	1:F:128:ALA:HB3	2.01	0.42
1:F:157:LEU:HD13	1:F:205:LEU:HD22	2.01	0.42
1:B:119:ILE:O	1:B:147:CYS:HA	2.20	0.42
1:A:218:GLN:HE21	1:A:218:GLN:HB3	1.65	0.42
1:C:76:TYR:HD1	1:C:79:LEU:HD12	1.85	0.42
1:F:91:ILE:HB	1:F:124:GLY:HA3	2.01	0.42
1:C:91:ILE:O	1:C:125:VAL:N	2.52	0.42
1:C:166:MET:O	1:C:168:HIS:CE1	2.72	0.42
1:E:91:ILE:O	1:E:124:GLY:HA3	2.20	0.42
1:E:148:VAL:HG11	2:E:301:OY9:C02	2.50	0.42
1:A:117:MET:HE3	1:A:143:ILE:HG21	2.01	0.42
1:F:101:ALA:HB1	1:G:75:ILE:HG12	2.00	0.42
1:G:159:LEU:HD21	1:G:241:LEU:HD21	2.02	0.42
1:D:209:TYR:HB3	1:D:220:ILE:HD12	2.02	0.41
1:F:248:PRO:HA	1:F:249:PRO:HD2	1.85	0.41
1:B:116:HIS:CE1	1:B:144:CYS:SG	3.14	0.41
1:C:107:GLN:HE21	1:C:107:GLN:HB3	1.65	0.41
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.81	0.41
1:A:153:SER:OG	1:A:154:MET:N	2.51	0.41
1:C:197:GLU:HB2	3:C:404:HOH:O	2.20	0.41
1:C:217:LEU:HD23	1:C:217:LEU:HA	1.91	0.41
1:D:97:SER:HB3	1:E:88:MET:HG3	2.02	0.41
1:B:111:ASN:OD1	1:B:111:ASN:N	2.52	0.41
1:F:100:ILE:HG23	1:F:135:THR:HG21	2.02	0.41
1:F:144[B]:CYS:SG	1:F:146:TRP:NE1	2.92	0.41
1:F:246:VAL:HG12	1:F:247:HIS:CE1	2.55	0.41
1:D:216:SER:N	3:D:401:HOH:O	2.43	0.41
1:C:242:ASP:C	1:C:243:LYS:HG3	2.41	0.41
1:G:231:SER:OG	1:G:234:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HA	1:B:220:ILE:HD13	1.86	0.41
1:G:118:TYR:OH	2:G:301:OY9:N09	2.54	0.41
1:G:129:GLY:HA3	1:G:154:MET:HE2	2.03	0.41
1:G:213:THR:HG22	1:G:239:GLY:C	2.42	0.41
1:C:63:VAL:O	1:C:63:VAL:HG23	2.21	0.40
1:D:78:ARG:O	1:D:81:ARG:HB3	2.21	0.40
1:F:73:TYR:OH	1:F:81:ARG:HD2	2.21	0.40
1:B:148:VAL:HG11	2:B:301:OY9:N01	2.36	0.40
1:C:191:ILE:HG12	3:C:410:HOH:O	2.21	0.40
1:G:104:LEU:HA	1:G:104:LEU:HD23	1.77	0.40
1:C:196:GLU:OE1	1:C:196:GLU:N	2.53	0.40
1:G:173:SER:O	1:G:232:PRO:HD3	2.21	0.40
1:F:201:LEU:HD23	1:F:204:GLN:OE1	2.22	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	170/221 (77%)	155 (91%)	14 (8%)	1 (1%)	25	61
1	B	172/221 (78%)	157 (91%)	14 (8%)	1 (1%)	25	61
1	C	172/221 (78%)	150 (87%)	21 (12%)	1 (1%)	25	61
1	D	173/221 (78%)	162 (94%)	8 (5%)	3 (2%)	9	39
1	E	173/221 (78%)	162 (94%)	10 (6%)	1 (1%)	25	61
1	F	176/221 (80%)	162 (92%)	12 (7%)	2 (1%)	14	48
1	G	172/221 (78%)	158 (92%)	11 (6%)	3 (2%)	9	39
All	All	1208/1547 (78%)	1106 (92%)	90 (8%)	12 (1%)	15	50

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	193	ILE
1	F	110	SER
1	G	190	ASP
1	G	246	VAL
1	A	125	VAL
1	B	190	ASP
1	C	193	ILE
1	E	191	ILE
1	F	82	GLU
1	D	192	ALA
1	D	191	ILE
1	G	122	PRO

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	153/185 (83%)	150 (98%)	3 (2%)	55	78
1	B	154/185 (83%)	152 (99%)	2 (1%)	69	85
1	C	155/185 (84%)	154 (99%)	1 (1%)	86	93
1	D	156/185 (84%)	155 (99%)	1 (1%)	86	93
1	E	155/185 (84%)	153 (99%)	2 (1%)	69	85
1	F	158/185 (85%)	156 (99%)	2 (1%)	69	85
1	G	155/185 (84%)	154 (99%)	1 (1%)	86	93
All	All	1086/1295 (84%)	1074 (99%)	12 (1%)	73	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	117	MET
1	A	218	GLN
1	B	97	SER
1	B	117	MET
1	C	81	ARG

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Mol	Chain	Res	Type
1	D	97	SER
1	E	63	VAL
1	E	88	MET
1	F	88	MET
1	F	190	ASP
1	G	174	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	120	ASN
1	A	218	GLN
1	B	204	GLN
1	C	107	GLN
1	C	172	ASN
1	C	207	ASN
1	D	179	GLN
1	E	168	HIS
1	E	236	GLN
1	F	150	GLN
1	F	218	GLN
1	F	236	GLN
1	G	116	HIS
1	G	168	HIS
1	G	236	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	OY9	B	301	-	31,31,31	3.70	11 (35%)	37,43,43	2.03	14 (37%)
2	OY9	C	301	-	31,31,31	3.38	13 (41%)	37,43,43	2.32	13 (35%)
2	OY9	G	301	-	31,31,31	3.74	12 (38%)	37,43,43	2.34	14 (37%)
2	OY9	E	301	-	31,31,31	3.54	11 (35%)	37,43,43	2.11	10 (27%)
2	OY9	F	301	-	31,31,31	3.65	11 (35%)	37,43,43	2.15	11 (29%)
2	OY9	A	301	-	31,31,31	3.43	11 (35%)	37,43,43	1.90	9 (24%)
2	OY9	D	301	-	31,31,31	3.72	10 (32%)	37,43,43	2.22	12 (32%)

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	OY9	B	301	-	-	0/10/19/19	0/4/4/4
2	OY9	C	301	-	-	2/10/19/19	0/4/4/4
2	OY9	G	301	-	-	2/10/19/19	0/4/4/4
2	OY9	E	301	-	-	1/10/19/19	0/4/4/4
2	OY9	F	301	-	-	0/10/19/19	0/4/4/4
2	OY9	A	301	-	-	1/10/19/19	0/4/4/4
2	OY9	D	301	-	-	2/10/19/19	0/4/4/4

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	OY9	C08-N09	-11.51	1.25	1.47
2	D	301	OY9	C08-N09	-11.04	1.26	1.47
2	F	301	OY9	C08-N09	-11.03	1.26	1.47
2	G	301	OY9	C08-N09	-10.99	1.26	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	OY9	C27-N09	-10.23	1.37	1.46
2	A	301	OY9	C08-N09	-10.21	1.27	1.47
2	C	301	OY9	C08-N09	-10.14	1.28	1.47
2	E	301	OY9	C08-N09	-10.13	1.28	1.47
2	G	301	OY9	C20-CL21	10.11	1.96	1.74
2	F	301	OY9	C27-N09	-9.83	1.37	1.46
2	G	301	OY9	C27-N09	-9.65	1.37	1.46
2	B	301	OY9	C27-N09	-9.48	1.38	1.46
2	D	301	OY9	C20-CL21	9.18	1.94	1.74
2	E	301	OY9	C20-CL21	9.05	1.94	1.74
2	C	301	OY9	C20-CL21	9.03	1.94	1.74
2	B	301	OY9	C20-CL21	8.63	1.93	1.74
2	A	301	OY9	C27-N09	-8.50	1.38	1.46
2	E	301	OY9	C27-N09	-8.48	1.38	1.46
2	F	301	OY9	C20-CL21	7.98	1.91	1.74
2	A	301	OY9	C20-CL21	7.94	1.91	1.74
2	C	301	OY9	C27-N09	-7.17	1.40	1.46
2	E	301	OY9	C24-N15	-6.66	1.29	1.39
2	B	301	OY9	C24-N15	-6.28	1.29	1.39
2	D	301	OY9	C24-N15	-5.88	1.30	1.39
2	G	301	OY9	C24-N15	-5.79	1.30	1.39
2	F	301	OY9	C24-N15	-5.47	1.30	1.39
2	A	301	OY9	C24-N15	-5.23	1.31	1.39
2	F	301	OY9	C03-C02	5.14	1.56	1.44
2	C	301	OY9	C24-N15	-5.08	1.31	1.39
2	B	301	OY9	C03-C02	4.90	1.55	1.44
2	D	301	OY9	C03-C02	4.75	1.55	1.44
2	A	301	OY9	C03-C02	4.53	1.54	1.44
2	A	301	OY9	C08-C07	4.40	1.59	1.51
2	E	301	OY9	C03-C02	4.40	1.54	1.44
2	G	301	OY9	C03-C02	4.30	1.54	1.44
2	F	301	OY9	C08-C07	4.05	1.58	1.51
2	C	301	OY9	C03-C02	3.98	1.53	1.44
2	B	301	OY9	C08-C07	3.61	1.57	1.51
2	F	301	OY9	C16-N15	3.42	1.53	1.47
2	A	301	OY9	C16-N15	3.41	1.53	1.47
2	E	301	OY9	C08-C07	3.34	1.57	1.51
2	D	301	OY9	C08-C07	3.22	1.57	1.51
2	C	301	OY9	C10-C11	3.16	1.60	1.52
2	C	301	OY9	C16-N15	3.15	1.52	1.47
2	G	301	OY9	C14-N15	-3.12	1.32	1.36
2	C	301	OY9	C08-C07	3.04	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	OY9	C10-C11	2.93	1.59	1.52
2	D	301	OY9	C16-N15	2.91	1.52	1.47
2	E	301	OY9	C14-N15	-2.91	1.33	1.36
2	E	301	OY9	C10-C11	2.85	1.59	1.52
2	E	301	OY9	C16-N15	2.78	1.52	1.47
2	G	301	OY9	C08-C07	2.75	1.56	1.51
2	G	301	OY9	C16-N15	2.72	1.52	1.47
2	F	301	OY9	C10-C11	2.70	1.59	1.52
2	B	301	OY9	C28-C07	2.69	1.43	1.39
2	F	301	OY9	C11-C12	2.64	1.55	1.50
2	B	301	OY9	C14-N15	-2.62	1.33	1.36
2	A	301	OY9	C10-C11	2.61	1.59	1.52
2	C	301	OY9	C27-C26	2.58	1.54	1.51
2	G	301	OY9	C26-C12	-2.50	1.32	1.37
2	G	301	OY9	C10-C11	2.49	1.58	1.52
2	A	301	OY9	C11-C12	2.45	1.54	1.50
2	D	301	OY9	C11-C12	2.42	1.54	1.50
2	C	301	OY9	C28-C07	2.41	1.43	1.39
2	F	301	OY9	C28-C07	2.38	1.43	1.39
2	D	301	OY9	C28-C07	2.36	1.43	1.39
2	A	301	OY9	C28-C07	2.32	1.43	1.39
2	E	301	OY9	C26-C12	-2.28	1.32	1.37
2	B	301	OY9	C10-C11	2.25	1.58	1.52
2	G	301	OY9	C02-N01	-2.23	1.09	1.14
2	B	301	OY9	C10-N09	-2.21	1.40	1.46
2	A	301	OY9	C27-C26	2.20	1.54	1.51
2	C	301	OY9	C14-N15	-2.18	1.34	1.36
2	C	301	OY9	C02-N01	-2.18	1.09	1.14
2	B	301	OY9	C16-N15	2.13	1.51	1.47
2	C	301	OY9	C11-C12	2.10	1.54	1.50
2	F	301	OY9	C27-C26	2.04	1.54	1.51
2	E	301	OY9	C11-C12	2.03	1.54	1.50
2	G	301	OY9	C28-C07	2.01	1.42	1.39

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	OY9	N15-C14-N13	-6.55	119.96	126.46
2	G	301	OY9	C16-N15-C24	6.13	123.72	117.61
2	D	301	OY9	C08-N09-C27	-5.92	102.75	110.53
2	E	301	OY9	C11-C10-N09	5.65	116.36	111.23
2	G	301	OY9	C11-C10-N09	5.60	116.31	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	OY9	C27-N09-C10	5.48	117.06	109.95
2	E	301	OY9	N15-C14-N13	-5.45	121.06	126.46
2	B	301	OY9	N15-C14-N13	-5.32	121.19	126.46
2	C	301	OY9	C11-C10-N09	5.30	116.05	111.23
2	D	301	OY9	C11-C10-N09	5.10	115.86	111.23
2	C	301	OY9	C27-N09-C10	4.82	116.20	109.95
2	C	301	OY9	C16-N15-C24	4.78	122.38	117.61
2	C	301	OY9	N15-C14-N13	-4.74	121.77	126.46
2	G	301	OY9	N15-C14-N13	-4.64	121.86	126.46
2	A	301	OY9	C27-N09-C10	4.54	115.83	109.95
2	F	301	OY9	C17-C16-N15	-4.29	106.34	112.83
2	A	301	OY9	C16-N15-C24	4.15	121.74	117.61
2	A	301	OY9	N15-C14-N13	-4.10	122.39	126.46
2	G	301	OY9	O25-C24-C26	-4.07	117.32	125.08
2	C	301	OY9	C14-N15-C24	-4.06	120.12	123.08
2	D	301	OY9	N15-C14-N13	-3.82	122.67	126.46
2	A	301	OY9	C14-N15-C24	-3.68	120.41	123.08
2	G	301	OY9	C27-N09-C10	3.65	114.68	109.95
2	D	301	OY9	C16-N15-C24	3.63	121.23	117.61
2	B	301	OY9	C28-C03-C02	3.62	124.36	119.54
2	C	301	OY9	C07-C08-N09	-3.57	106.20	113.12
2	D	301	OY9	C27-N09-C10	3.51	114.50	109.95
2	E	301	OY9	C16-N15-C24	3.46	121.06	117.61
2	B	301	OY9	C16-N15-C24	3.43	121.03	117.61
2	F	301	OY9	C11-C12-N13	3.42	119.91	114.62
2	D	301	OY9	C11-C12-N13	3.35	119.81	114.62
2	D	301	OY9	C17-C16-N15	-3.32	107.81	112.83
2	E	301	OY9	C14-N15-C24	-3.30	120.68	123.08
2	D	301	OY9	O25-C24-C26	-3.28	118.82	125.08
2	G	301	OY9	C14-N15-C24	-3.08	120.84	123.08
2	D	301	OY9	C26-C12-N13	-3.04	119.26	123.68
2	A	301	OY9	C11-C12-N13	3.04	119.33	114.62
2	B	301	OY9	C04-C03-C02	-3.03	114.94	119.99
2	B	301	OY9	C17-C16-N15	-3.00	108.29	112.83
2	G	301	OY9	O25-C24-N15	3.00	124.59	120.61
2	C	301	OY9	O25-C24-C26	-2.97	119.41	125.08
2	G	301	OY9	C08-N09-C27	-2.94	106.66	110.53
2	G	301	OY9	C08-N09-C10	-2.91	104.59	111.06
2	A	301	OY9	O25-C24-C26	-2.85	119.65	125.08
2	E	301	OY9	C26-C24-N15	2.84	120.14	115.20
2	E	301	OY9	C23-C17-C18	2.83	122.61	118.17
2	E	301	OY9	C27-N09-C10	2.81	113.60	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	OY9	O25-C24-N15	2.74	124.25	120.61
2	C	301	OY9	C26-C24-N15	2.71	119.91	115.20
2	E	301	OY9	C26-C12-N13	-2.70	119.75	123.68
2	B	301	OY9	C08-C07-C06	-2.68	115.72	120.77
2	D	301	OY9	C14-N15-C24	-2.65	121.15	123.08
2	G	301	OY9	C26-C12-N13	-2.65	119.83	123.68
2	E	301	OY9	O25-C24-C26	-2.62	120.08	125.08
2	B	301	OY9	C23-C17-C18	2.61	122.27	118.17
2	B	301	OY9	C27-N09-C10	2.61	113.33	109.95
2	F	301	OY9	O25-C24-C26	-2.57	120.17	125.08
2	F	301	OY9	C26-C24-N15	2.54	119.61	115.20
2	C	301	OY9	C26-C12-N13	-2.51	120.03	123.68
2	A	301	OY9	C26-C12-N13	-2.50	120.05	123.68
2	C	301	OY9	C11-C12-N13	2.47	118.44	114.62
2	B	301	OY9	C11-C10-N09	-2.46	109.00	111.23
2	E	301	OY9	C11-C12-N13	2.41	118.35	114.62
2	F	301	OY9	C26-C12-N13	-2.40	120.19	123.68
2	F	301	OY9	C24-C26-C12	-2.39	117.14	119.35
2	G	301	OY9	C17-C16-N15	-2.36	109.26	112.83
2	F	301	OY9	C19-C20-CL21	-2.35	115.69	119.35
2	B	301	OY9	C08-N09-C10	-2.35	105.84	111.06
2	C	301	OY9	C19-C20-CL21	2.30	122.94	119.35
2	B	301	OY9	C26-C12-N13	-2.29	120.34	123.68
2	A	301	OY9	C26-C24-N15	2.28	119.16	115.20
2	B	301	OY9	C11-C12-N13	2.27	118.14	114.62
2	G	301	OY9	C22-C20-C19	-2.26	118.31	121.24
2	F	301	OY9	C23-C17-C18	2.24	121.69	118.17
2	B	301	OY9	C26-C24-N15	2.20	119.02	115.20
2	G	301	OY9	C06-C07-C28	2.15	121.55	118.54
2	A	301	OY9	C19-C20-CL21	-2.13	116.03	119.35
2	B	301	OY9	C08-C07-C28	2.12	124.33	120.25
2	C	301	OY9	C24-C26-C12	-2.09	117.42	119.35
2	F	301	OY9	C18-C19-C20	-2.09	117.04	119.24
2	G	301	OY9	C18-C19-C20	2.09	121.45	119.24
2	D	301	OY9	C06-C07-C28	2.02	121.37	118.54
2	C	301	OY9	C17-C16-N15	-2.00	109.80	112.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	OY9	C07-C08-N09-C27

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Mol	Chain	Res	Type	Atoms
2	D	301	OY9	C07-C08-N09-C10
2	C	301	OY9	C07-C08-N09-C10
2	C	301	OY9	C07-C08-N09-C27
2	G	301	OY9	C07-C08-N09-C27
2	G	301	OY9	C07-C08-N09-C10
2	A	301	OY9	C07-C08-N09-C10
2	E	301	OY9	C07-C08-N09-C10

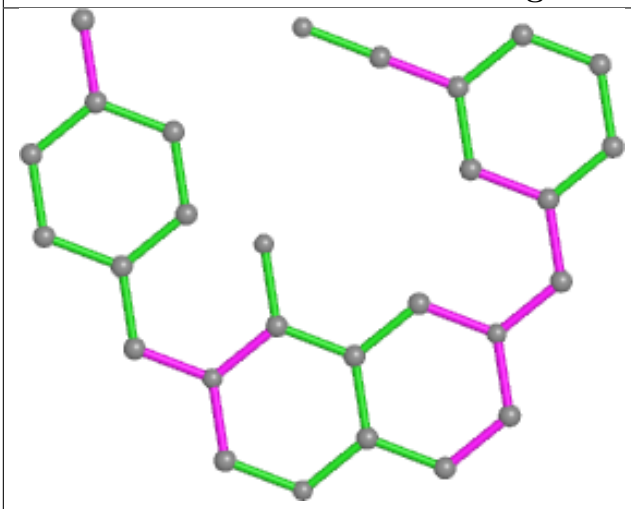
There are no ring outliers.

4 monomers are involved in 7 short contacts:

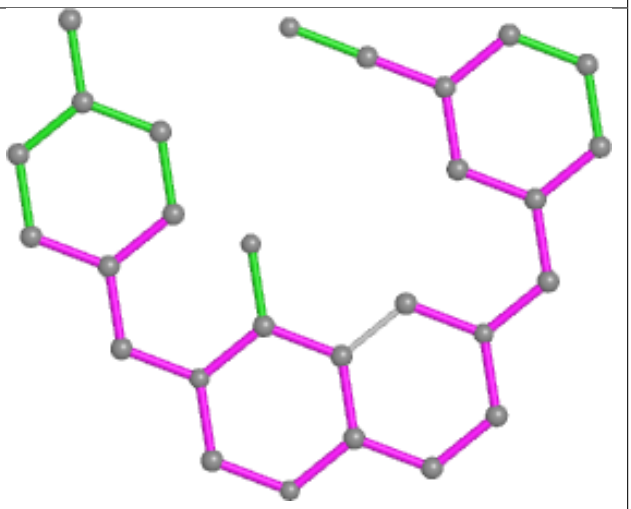
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	OY9	1	0
2	G	301	OY9	3	0
2	E	301	OY9	2	0
2	F	301	OY9	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

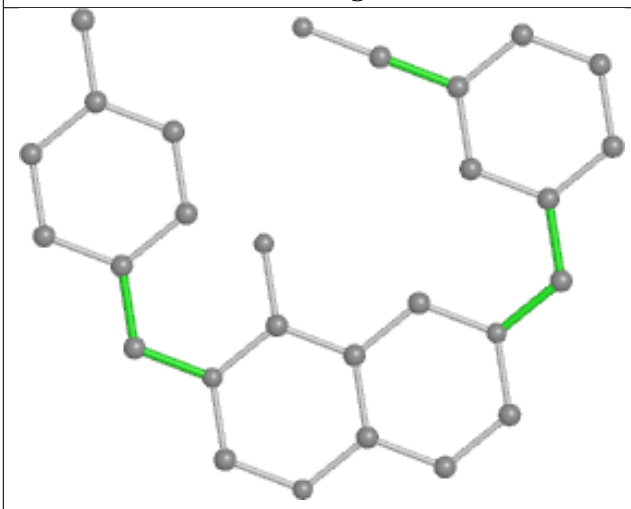
Ligand OY9 B 301



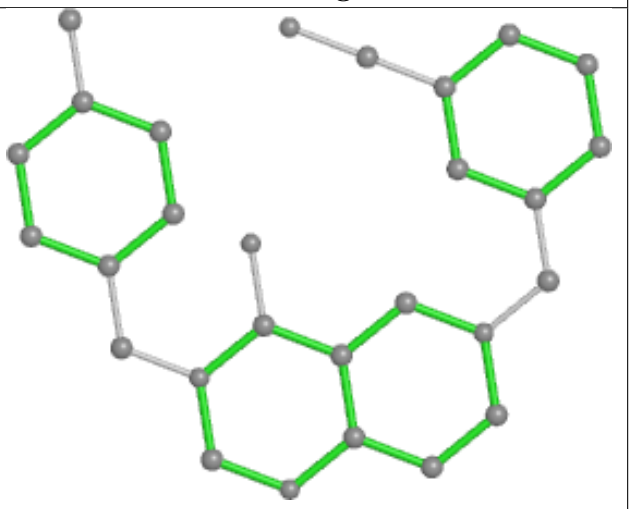
Bond lengths



Bond angles

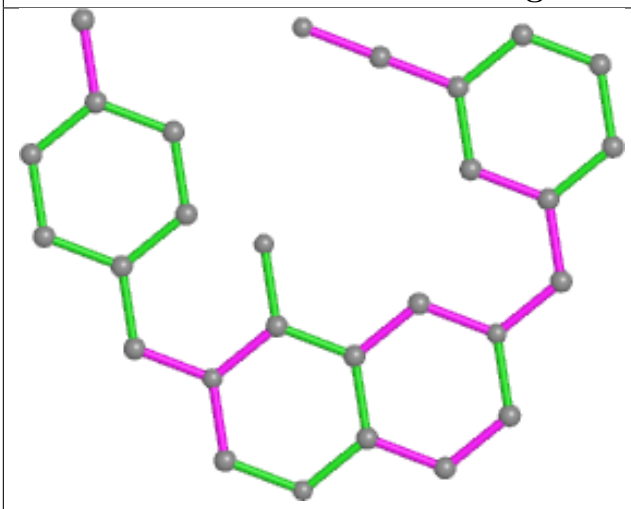


Torsions

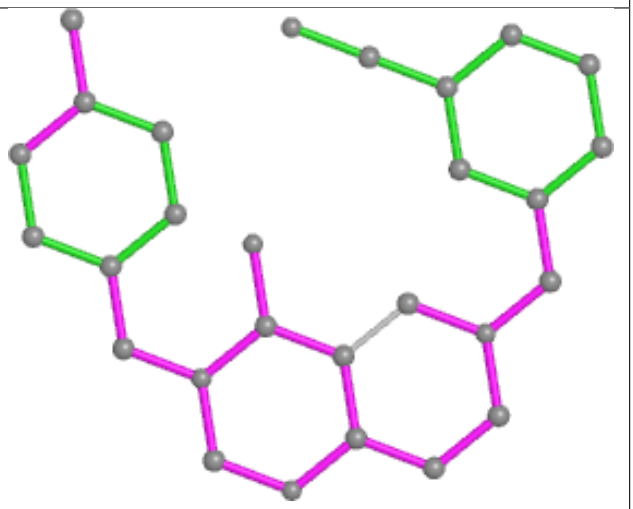


Rings

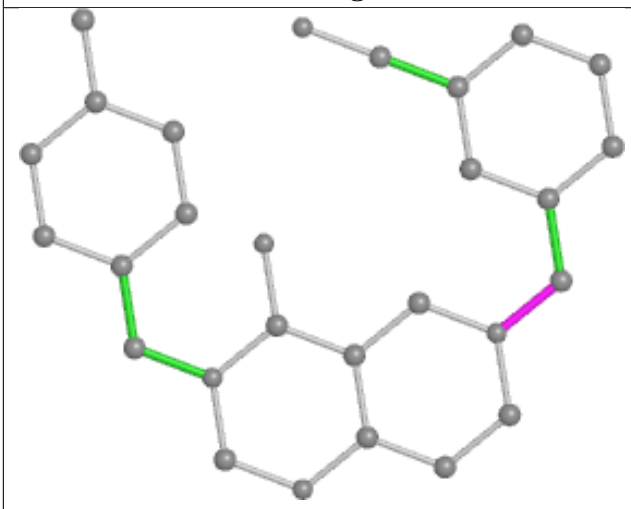
Ligand OY9 C 301



Bond lengths



Bond angles



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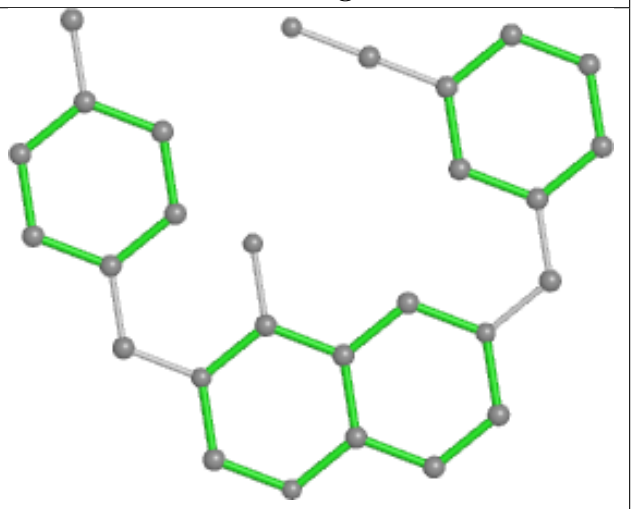
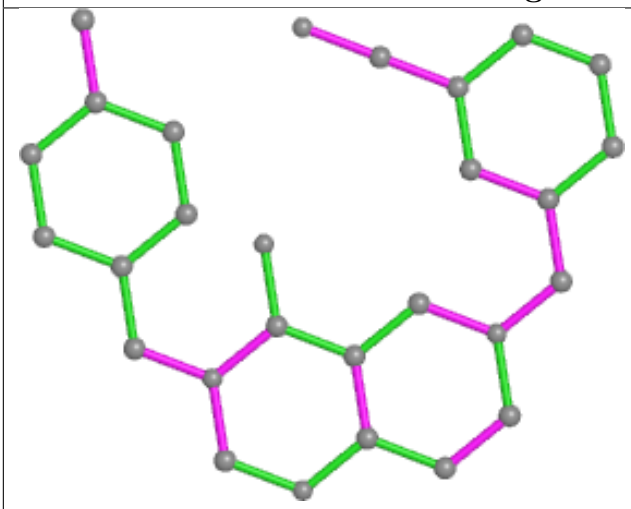
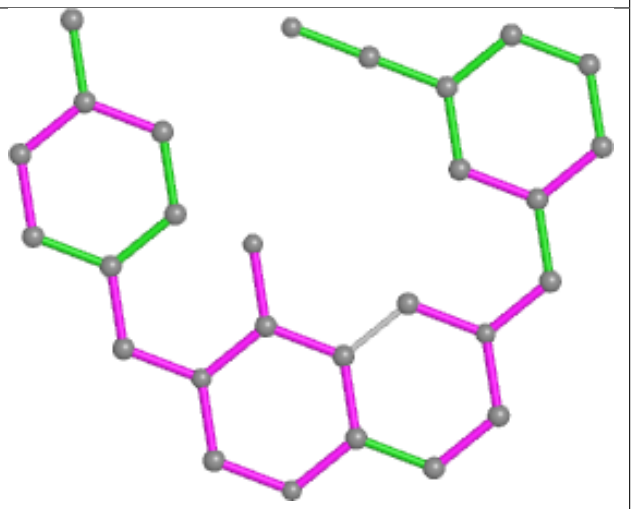


Rings

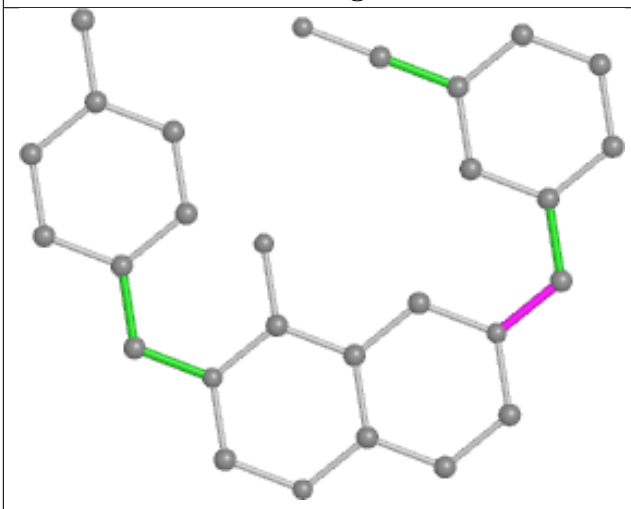
Ligand OY9 G 301



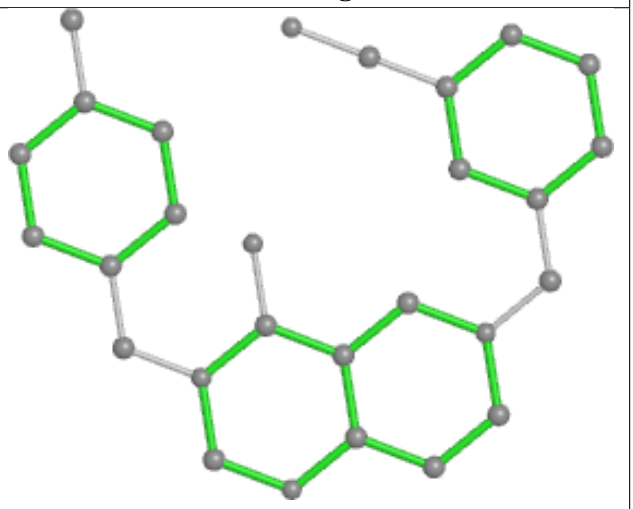
Bond lengths



Bond angles

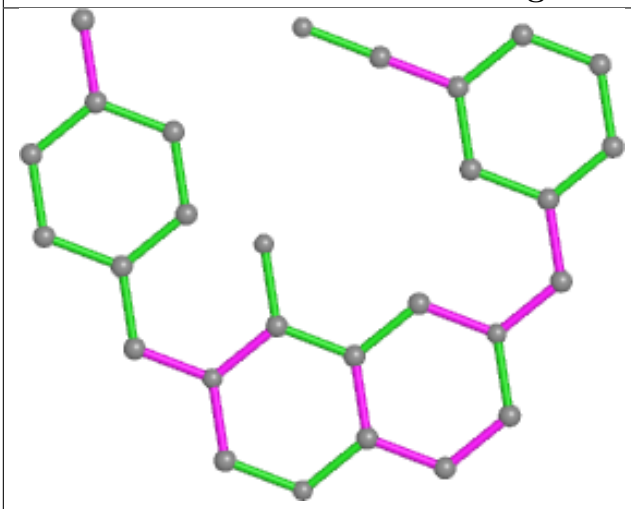


Torsions

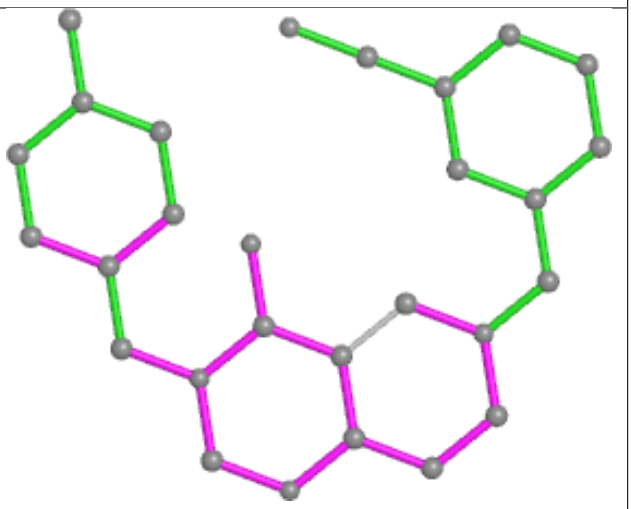


Rings

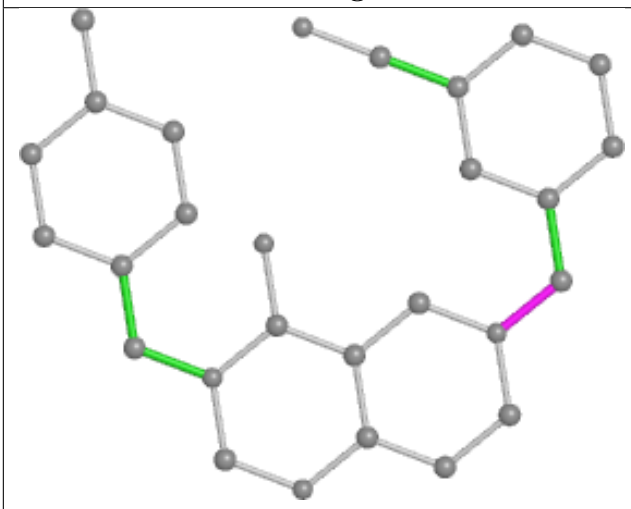
Ligand OY9 E 301



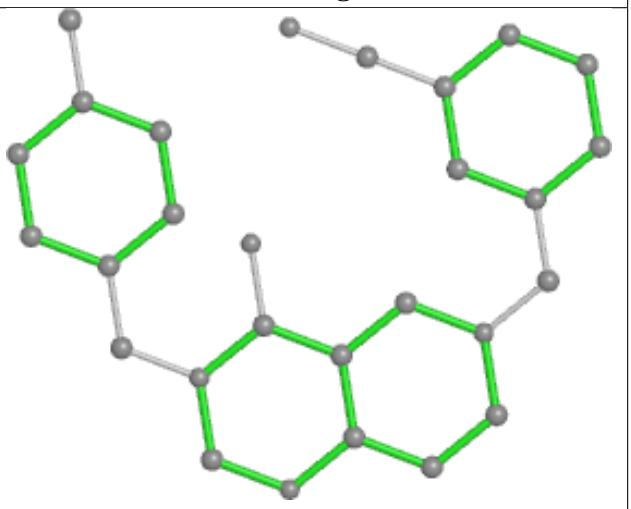
Bond lengths



Bond angles

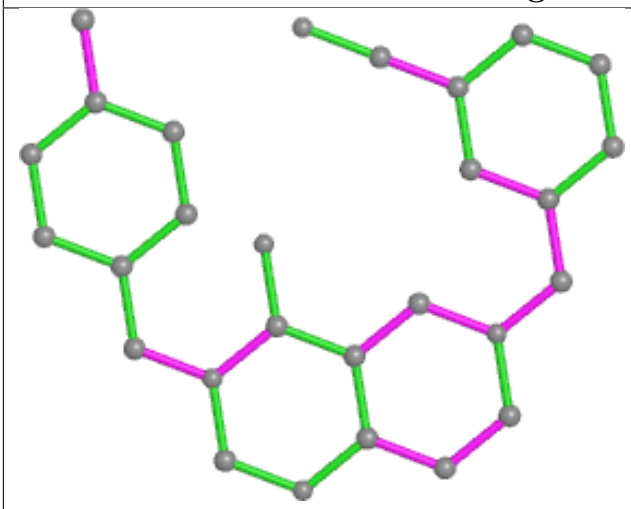


Torsions

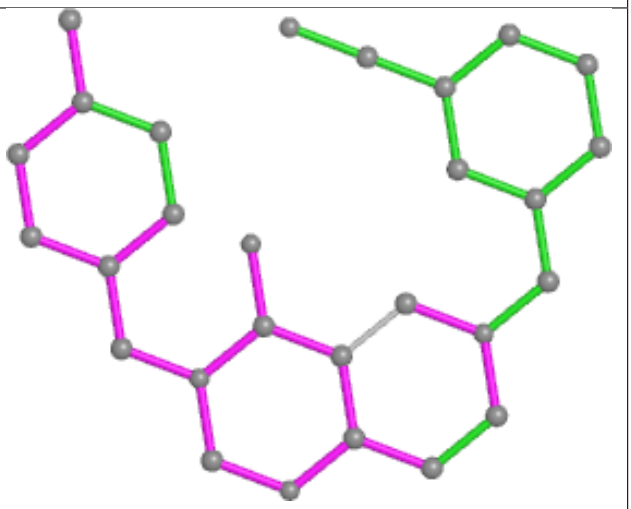


Rings

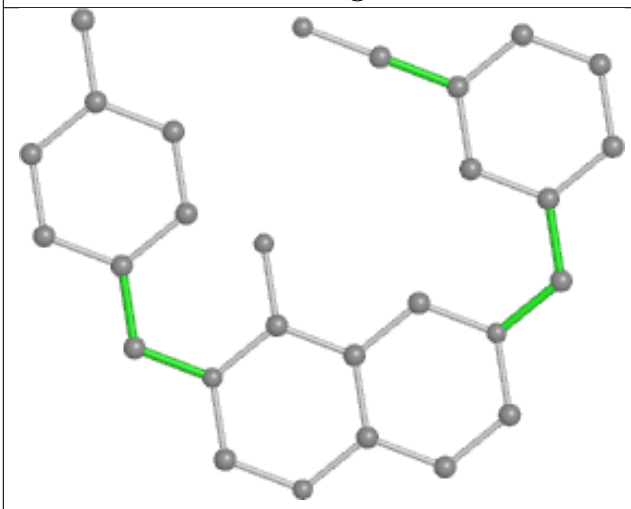
Ligand OY9 F 301



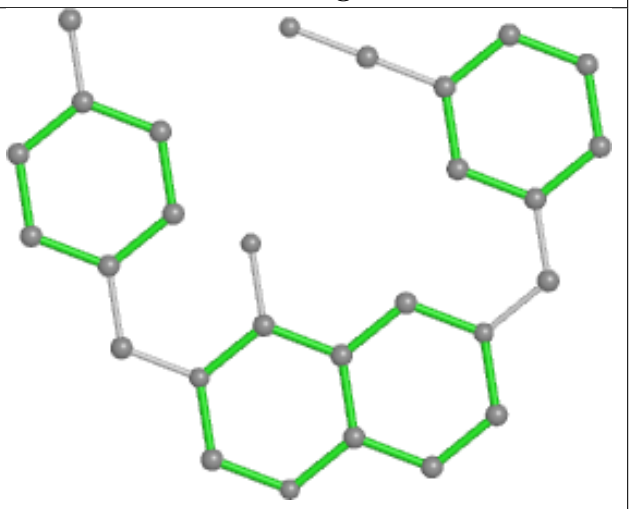
Bond lengths



Bond angles

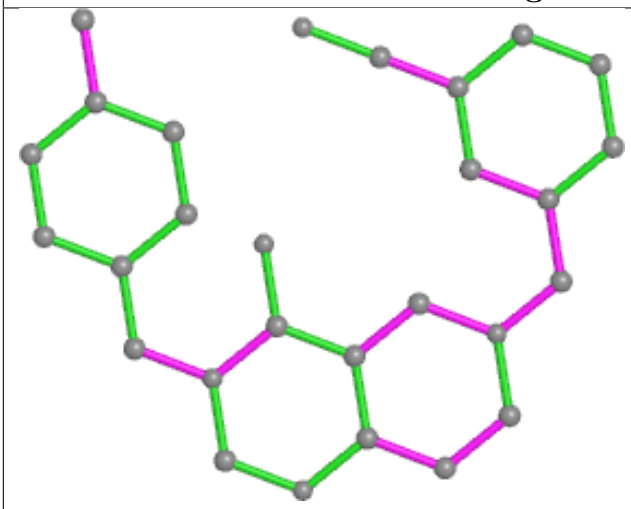


Torsions

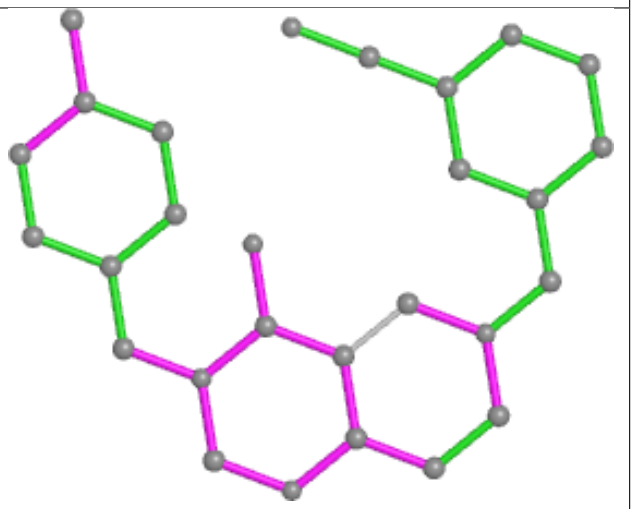


Rings

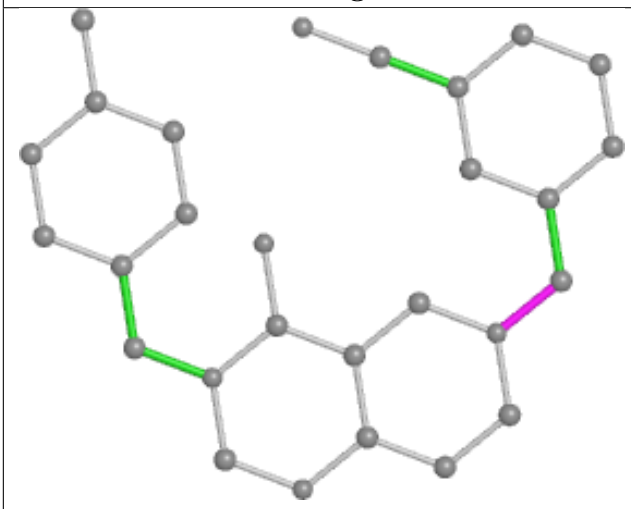
Ligand OY9 A 301



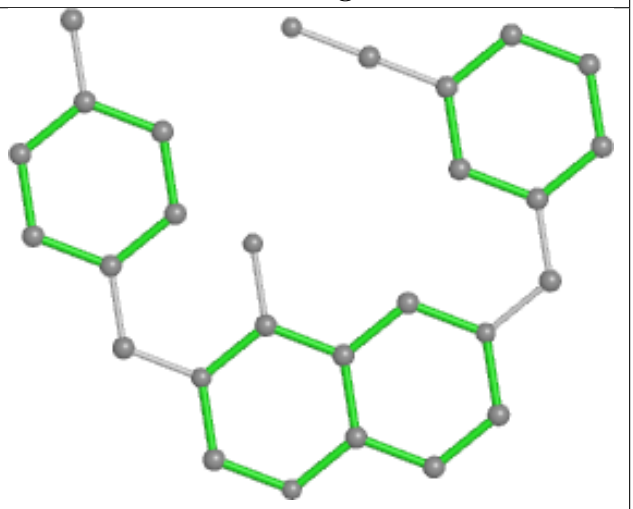
Bond lengths



Bond angles

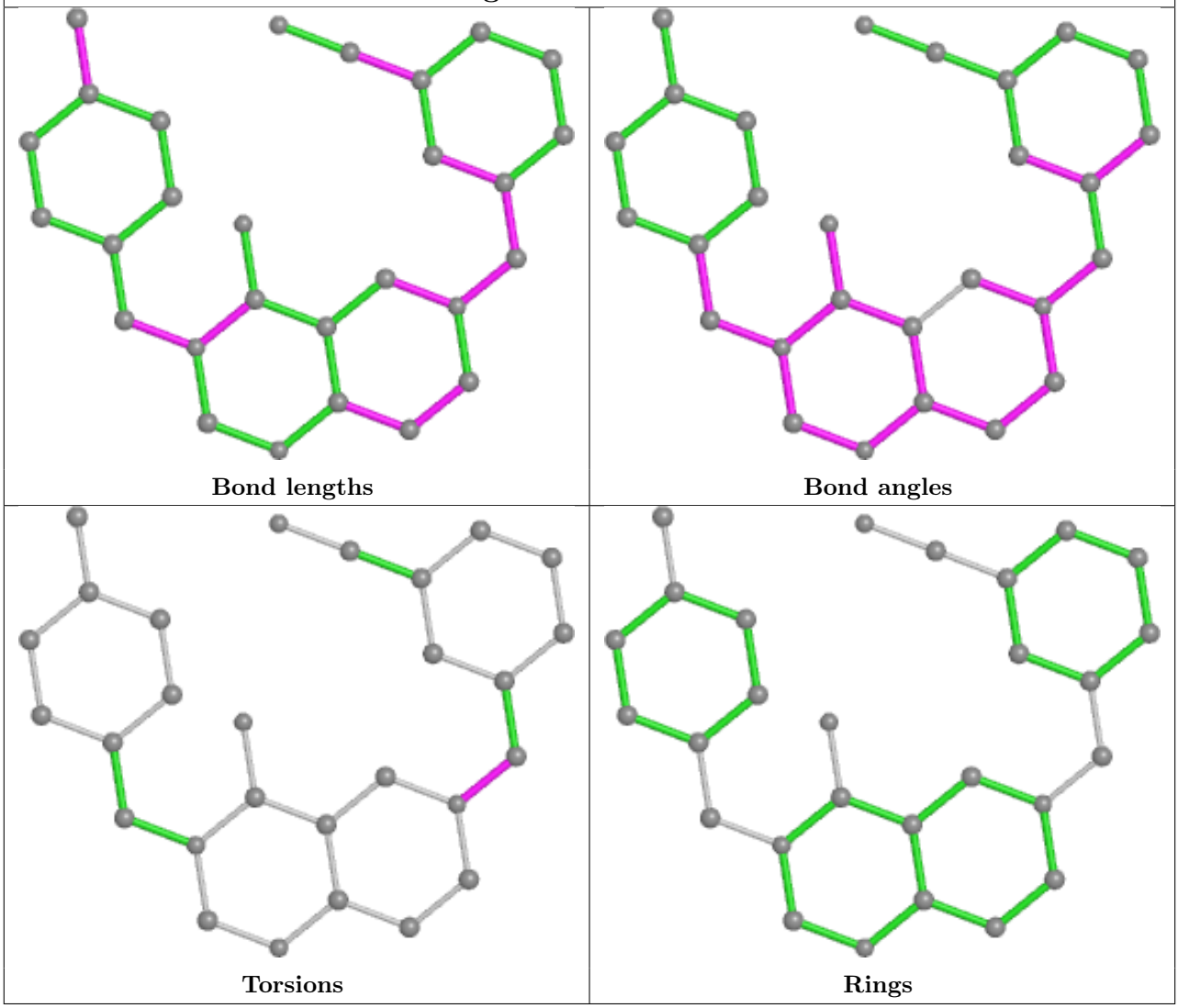


Torsions



Rings

Ligand OY9 D 301



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^{th} 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	176/221 (79%)	-0.42	1 (0%) 89 85	34, 44, 64, 92	0
1	B	178/221 (80%)	-0.28	0 100 100	37, 48, 69, 83	0
1	C	178/221 (80%)	-0.26	1 (0%) 89 85	30, 48, 73, 103	0
1	D	179/221 (80%)	-0.40	1 (0%) 89 85	32, 45, 66, 102	0
1	E	179/221 (80%)	-0.15	1 (0%) 89 85	32, 46, 71, 88	0
1	F	181/221 (81%)	-0.42	1 (0%) 89 85	33, 44, 67, 83	0
1	G	178/221 (80%)	-0.08	2 (1%) 80 73	35, 47, 71, 90	0
All	All	1249/1547 (80%)	-0.29	7 (0%) 89 85	30, 46, 70, 103	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	190	ASP	3.2
1	G	191	ILE	3.1
1	C	71	ARG	2.5
1	F	63	VAL	2.1
1	A	64	GLU	2.1
1	D	191	ILE	2.1
1	E	190	ASP	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

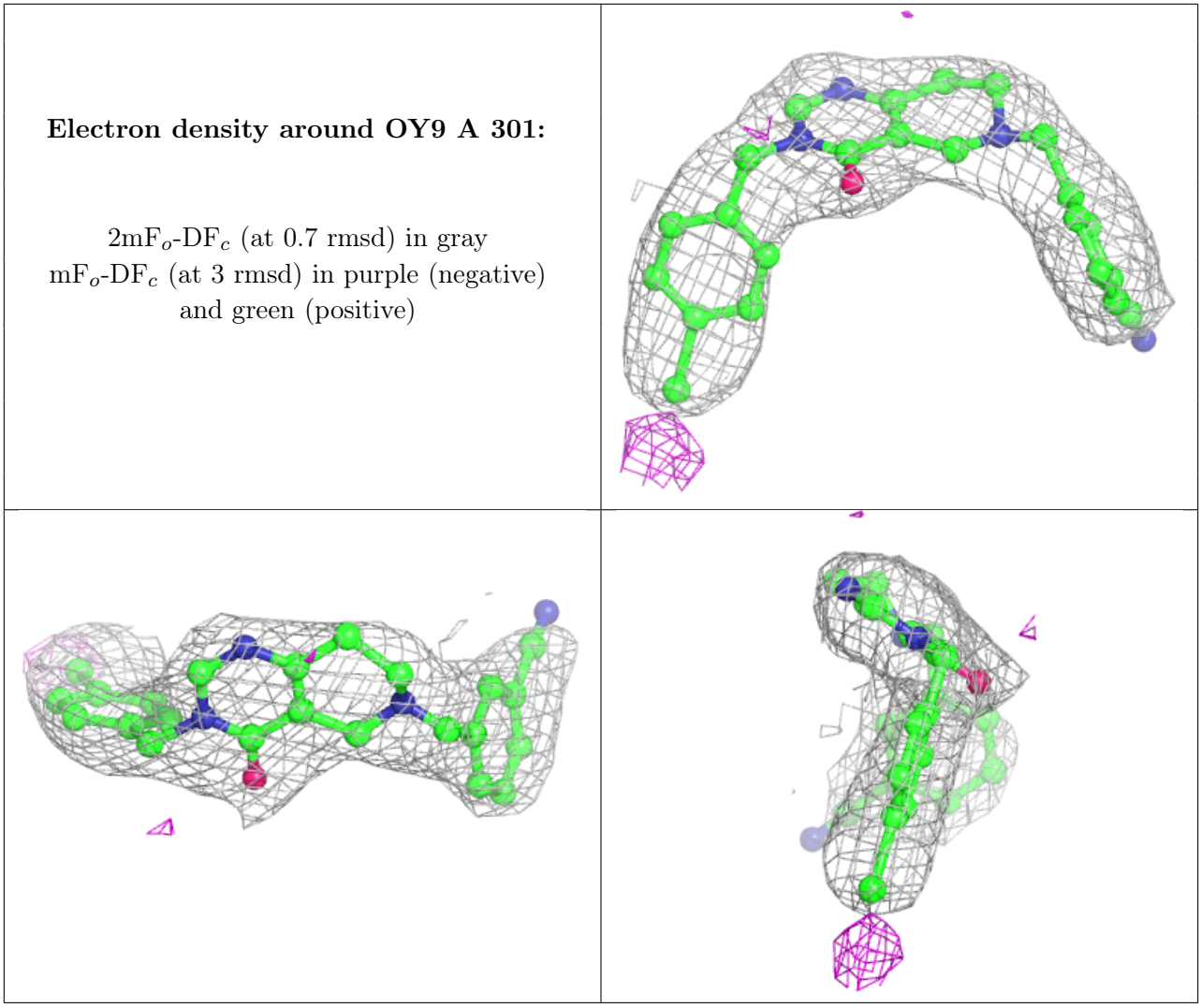
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	OY9	A	301	28/28	0.95	0.25	38,45,54,61	0
2	OY9	F	301	28/28	0.95	0.26	38,44,54,56	0
2	OY9	G	301	28/28	0.95	0.25	38,46,54,62	0
2	OY9	D	301	28/28	0.96	0.23	41,47,55,63	0
2	OY9	B	301	28/28	0.96	0.25	45,50,56,60	0
2	OY9	C	301	28/28	0.96	0.33	44,51,57,59	0
2	OY9	E	301	28/28	0.97	0.19	40,44,48,57	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.

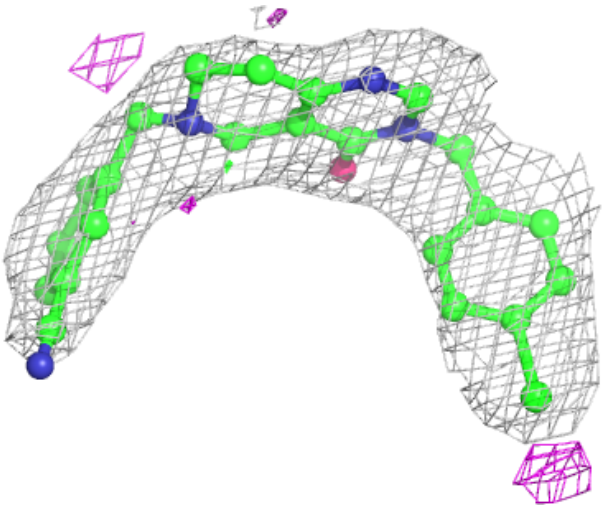
Electron density around OY9 A 301:

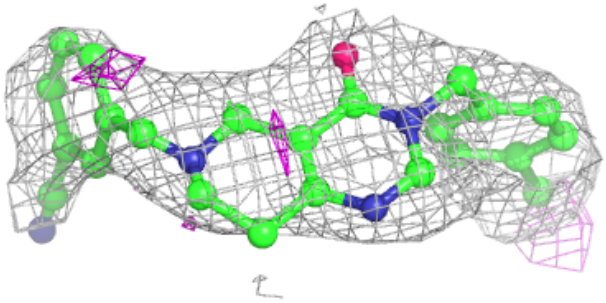
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

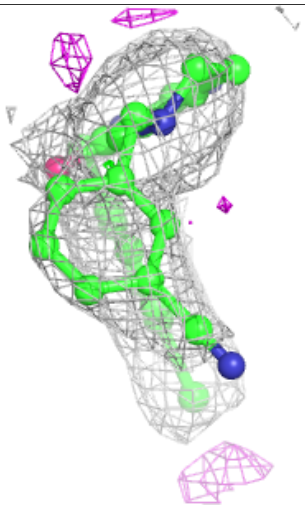


Electron density around OY9 F 301:

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

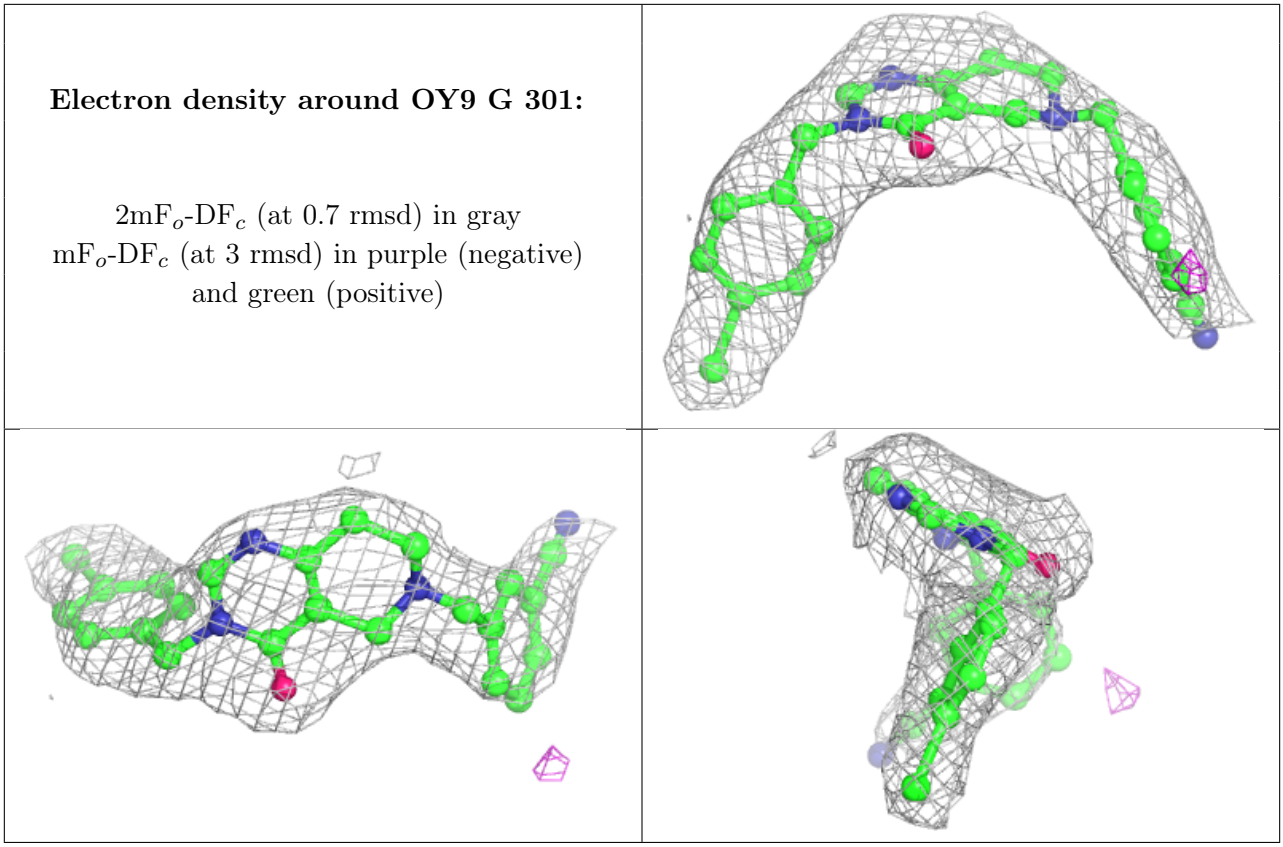






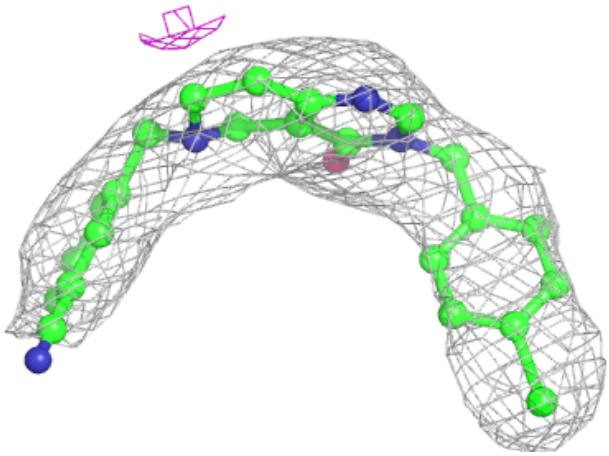
Electron density around OY9 G 301:

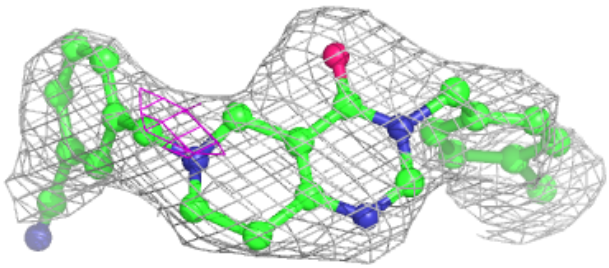
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

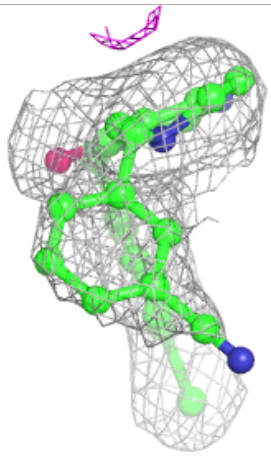


Electron density around OY9 D 301:

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

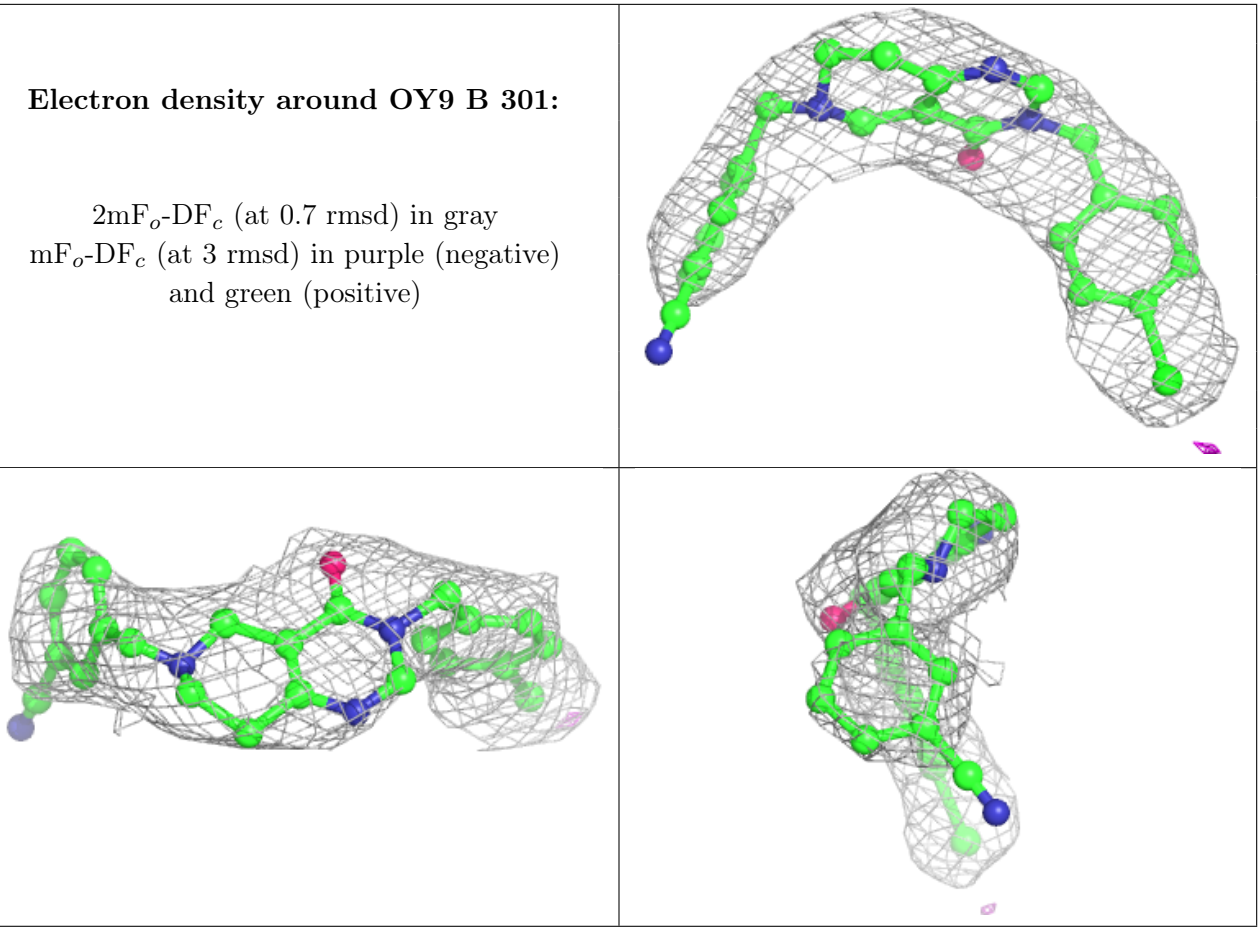






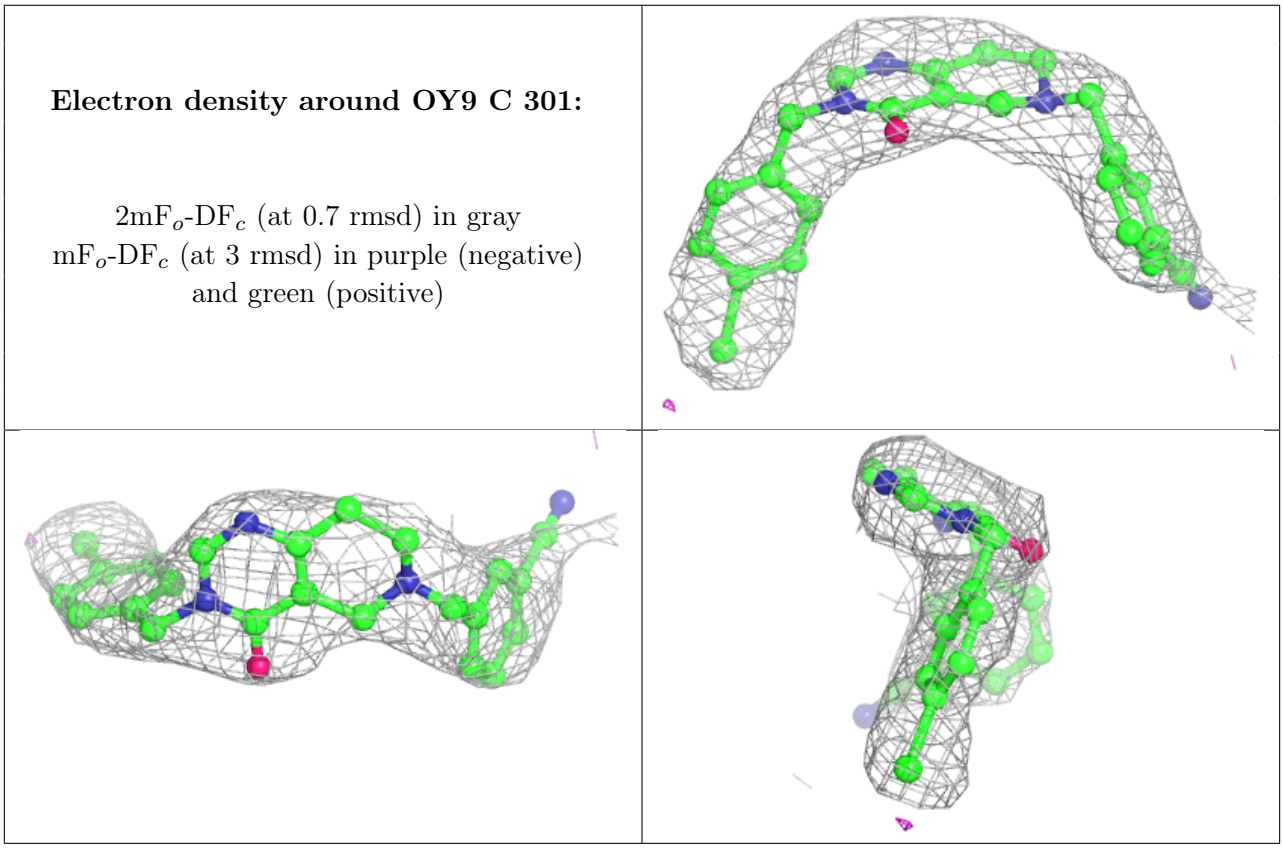
Electron density around OY9 B 301:

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



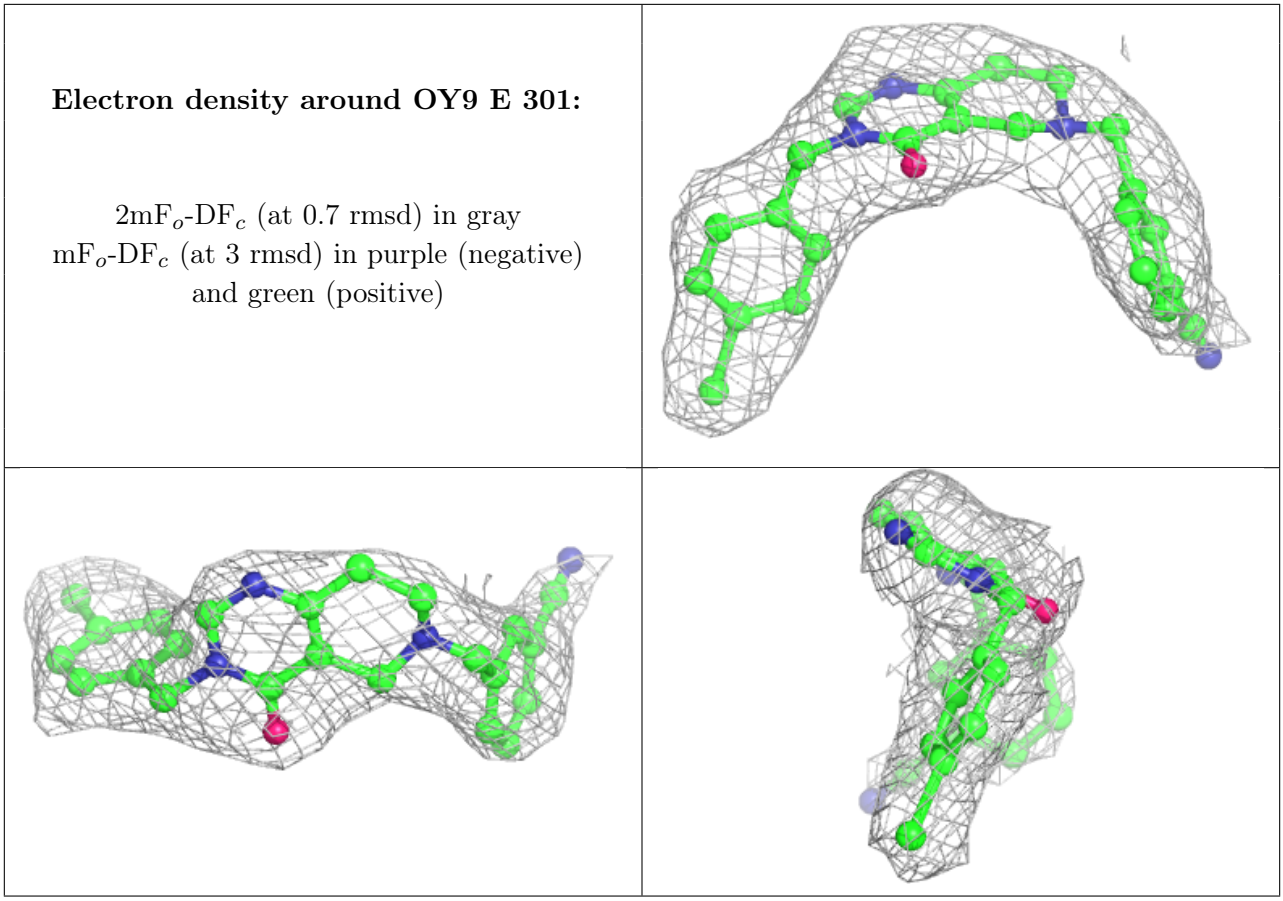
Electron density around OY9 C 301:

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



Electron density around OY9 E 301:

$2mF_o$-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

There are no such residues in this entry.