wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 06:29 pm GMT

PDB ID	:	5OBG
Title	:	Crystal structure of glycine binding protein in complex with strychnine
Authors	:	Dawson, A.; Hunter, W.N.; Jones, M.
Deposited on	:	2017-06-26
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

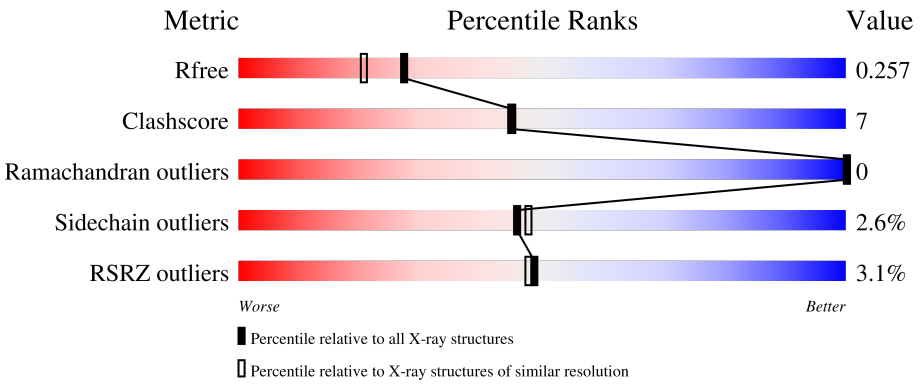
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	249	2%, 72%, 9%, •, 17%
1	B	249	2%, 74%, 8%, •, 16%
1	C	249	3%, 72%, 9%, •, 17%
1	D	249	2%, 74%, 8%, 17%
1	E	249	4%, 77%, 8%, 15%

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	SY9	C	601[B]	-	-	X	-
3	EDO	B	610	-	-	X	-
3	EDO	C	602	-	-	X	-
5	ACT	A	610	-	-	X	-
5	ACT	B	608	-	-	X	-
5	ACT	C	603	-	X	X	-
5	ACT	C	610	-	-	X	-
5	ACT	E	602	-	-	X	-
6	NAG	B	602	-	-	-	X
6	NAG	C	604	-	-	-	X
6	NAG	D	602	-	-	-	X
6	NAG	E	605	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9478 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1661	1050	277	327	7	0	2	0
1	B	208	1675	1064	275	328	8	0	2	0
1	C	206	1672	1059	279	327	7	0	3	0
1	D	206	1648	1042	273	326	7	0	0	0
1	E	212	1702	1078	283	334	7	0	3	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	PHE	THR	engineered mutation	UNP Q8WSF8
A	60	VAL	ALA	conflict	UNP Q8WSF8
A	74	ARG	GLN	engineered mutation	UNP Q8WSF8
A	110	ALA	TYR	engineered mutation	UNP Q8WSF8
A	135	SER	ILE	engineered mutation	UNP Q8WSF8
A	155	VAL	ALA	conflict	UNP Q8WSF8
A	162	GLU	GLY	engineered mutation	UNP Q8WSF8
A	206	LYS	SER	engineered mutation	UNP Q8WSF8
A	207	GLY	CYS	engineered mutation	UNP Q8WSF8
A	208	THR	CYS	engineered mutation	UNP Q8WSF8
A	209	GLY	PRO	engineered mutation	UNP Q8WSF8
A	237	GLU	-	expression tag	UNP Q8WSF8
A	238	ASN	-	expression tag	UNP Q8WSF8
A	239	LEU	-	expression tag	UNP Q8WSF8
A	240	TYR	-	expression tag	UNP Q8WSF8
A	241	PHE	-	expression tag	UNP Q8WSF8
A	242	GLN	-	expression tag	UNP Q8WSF8
A	243	GLY	-	expression tag	UNP Q8WSF8
A	244	HIS	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	HIS	-	expression tag	UNP Q8WSF8
A	246	HIS	-	expression tag	UNP Q8WSF8
A	247	HIS	-	expression tag	UNP Q8WSF8
A	248	HIS	-	expression tag	UNP Q8WSF8
A	249	HIS	-	expression tag	UNP Q8WSF8
B	53	PHE	THR	engineered mutation	UNP Q8WSF8
B	60	VAL	ALA	conflict	UNP Q8WSF8
B	74	ARG	GLN	engineered mutation	UNP Q8WSF8
B	110	ALA	TYR	engineered mutation	UNP Q8WSF8
B	135	SER	ILE	engineered mutation	UNP Q8WSF8
B	155	VAL	ALA	conflict	UNP Q8WSF8
B	162	GLU	GLY	engineered mutation	UNP Q8WSF8
B	206	LYS	SER	engineered mutation	UNP Q8WSF8
B	207	GLY	CYS	engineered mutation	UNP Q8WSF8
B	208	THR	CYS	engineered mutation	UNP Q8WSF8
B	209	GLY	PRO	engineered mutation	UNP Q8WSF8
B	237	GLU	-	expression tag	UNP Q8WSF8
B	238	ASN	-	expression tag	UNP Q8WSF8
B	239	LEU	-	expression tag	UNP Q8WSF8
B	240	TYR	-	expression tag	UNP Q8WSF8
B	241	PHE	-	expression tag	UNP Q8WSF8
B	242	GLN	-	expression tag	UNP Q8WSF8
B	243	GLY	-	expression tag	UNP Q8WSF8
B	244	HIS	-	expression tag	UNP Q8WSF8
B	245	HIS	-	expression tag	UNP Q8WSF8
B	246	HIS	-	expression tag	UNP Q8WSF8
B	247	HIS	-	expression tag	UNP Q8WSF8
B	248	HIS	-	expression tag	UNP Q8WSF8
B	249	HIS	-	expression tag	UNP Q8WSF8
C	53	PHE	THR	engineered mutation	UNP Q8WSF8
C	60	VAL	ALA	conflict	UNP Q8WSF8
C	74	ARG	GLN	engineered mutation	UNP Q8WSF8
C	110	ALA	TYR	engineered mutation	UNP Q8WSF8
C	135	SER	ILE	engineered mutation	UNP Q8WSF8
C	155	VAL	ALA	conflict	UNP Q8WSF8
C	162	GLU	GLY	engineered mutation	UNP Q8WSF8
C	206	LYS	SER	engineered mutation	UNP Q8WSF8
C	207	GLY	CYS	engineered mutation	UNP Q8WSF8
C	208	THR	CYS	engineered mutation	UNP Q8WSF8
C	209	GLY	PRO	engineered mutation	UNP Q8WSF8
C	237	GLU	-	expression tag	UNP Q8WSF8
C	238	ASN	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

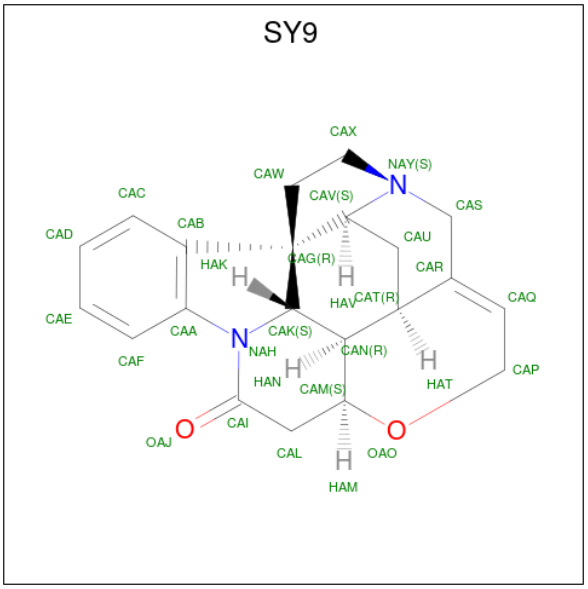
Chain	Residue	Modelled	Actual	Comment	Reference
C	239	LEU	-	expression tag	UNP Q8WSF8
C	240	TYR	-	expression tag	UNP Q8WSF8
C	241	PHE	-	expression tag	UNP Q8WSF8
C	242	GLN	-	expression tag	UNP Q8WSF8
C	243	GLY	-	expression tag	UNP Q8WSF8
C	244	HIS	-	expression tag	UNP Q8WSF8
C	245	HIS	-	expression tag	UNP Q8WSF8
C	246	HIS	-	expression tag	UNP Q8WSF8
C	247	HIS	-	expression tag	UNP Q8WSF8
C	248	HIS	-	expression tag	UNP Q8WSF8
C	249	HIS	-	expression tag	UNP Q8WSF8
D	53	PHE	THR	engineered mutation	UNP Q8WSF8
D	60	VAL	ALA	conflict	UNP Q8WSF8
D	74	ARG	GLN	engineered mutation	UNP Q8WSF8
D	110	ALA	TYR	engineered mutation	UNP Q8WSF8
D	135	SER	ILE	engineered mutation	UNP Q8WSF8
D	155	VAL	ALA	conflict	UNP Q8WSF8
D	162	GLU	GLY	engineered mutation	UNP Q8WSF8
D	206	LYS	SER	engineered mutation	UNP Q8WSF8
D	207	GLY	CYS	engineered mutation	UNP Q8WSF8
D	208	THR	CYS	engineered mutation	UNP Q8WSF8
D	209	GLY	PRO	engineered mutation	UNP Q8WSF8
D	237	GLU	-	expression tag	UNP Q8WSF8
D	238	ASN	-	expression tag	UNP Q8WSF8
D	239	LEU	-	expression tag	UNP Q8WSF8
D	240	TYR	-	expression tag	UNP Q8WSF8
D	241	PHE	-	expression tag	UNP Q8WSF8
D	242	GLN	-	expression tag	UNP Q8WSF8
D	243	GLY	-	expression tag	UNP Q8WSF8
D	244	HIS	-	expression tag	UNP Q8WSF8
D	245	HIS	-	expression tag	UNP Q8WSF8
D	246	HIS	-	expression tag	UNP Q8WSF8
D	247	HIS	-	expression tag	UNP Q8WSF8
D	248	HIS	-	expression tag	UNP Q8WSF8
D	249	HIS	-	expression tag	UNP Q8WSF8
E	53	PHE	THR	engineered mutation	UNP Q8WSF8
E	60	VAL	ALA	conflict	UNP Q8WSF8
E	74	ARG	GLN	engineered mutation	UNP Q8WSF8
E	110	ALA	TYR	engineered mutation	UNP Q8WSF8
E	135	SER	ILE	engineered mutation	UNP Q8WSF8
E	155	VAL	ALA	conflict	UNP Q8WSF8
E	162	GLU	GLY	engineered mutation	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	206	LYS	SER	engineered mutation	UNP Q8WSF8
E	207	GLY	CYS	engineered mutation	UNP Q8WSF8
E	208	THR	CYS	engineered mutation	UNP Q8WSF8
E	209	GLY	PRO	engineered mutation	UNP Q8WSF8
E	237	GLU	-	expression tag	UNP Q8WSF8
E	238	ASN	-	expression tag	UNP Q8WSF8
E	239	LEU	-	expression tag	UNP Q8WSF8
E	240	TYR	-	expression tag	UNP Q8WSF8
E	241	PHE	-	expression tag	UNP Q8WSF8
E	242	GLN	-	expression tag	UNP Q8WSF8
E	243	GLY	-	expression tag	UNP Q8WSF8
E	244	HIS	-	expression tag	UNP Q8WSF8
E	245	HIS	-	expression tag	UNP Q8WSF8
E	246	HIS	-	expression tag	UNP Q8WSF8
E	247	HIS	-	expression tag	UNP Q8WSF8
E	248	HIS	-	expression tag	UNP Q8WSF8
E	249	HIS	-	expression tag	UNP Q8WSF8

- Molecule 2 is STRYCHNINE (three-letter code: SY9) (formula: $C_{21}H_{22}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



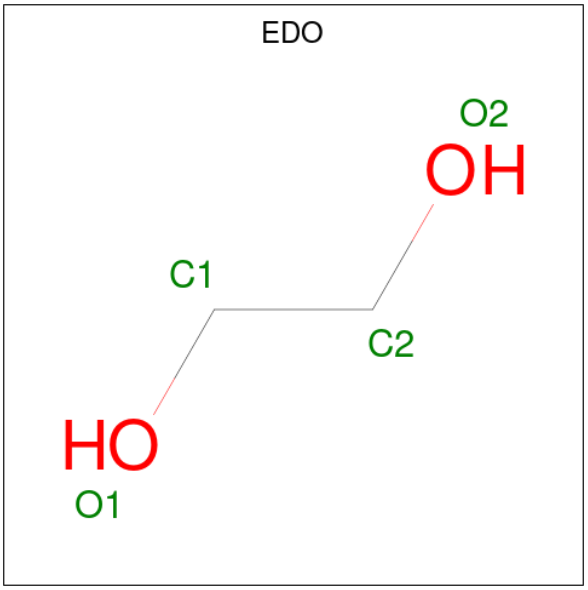
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	25	21	2	2	0	0
			Total	C	N	O		
2	B	1	25	21	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	50	42	4	4	0	1
			Total	C	N	O		
2	D	1	25	21	2	2	0	0
			Total	C	N	O		
2	E	1	25	21	2	2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	4	2	2		0	0
			Total	C	O			
3	A	1	4	2	2		0	0
			Total	C	O			
3	A	1	4	2	2		0	0
			Total	C	O			
3	A	1	4	2	2		0	0
			Total	C	O			
3	A	1	4	2	2		0	0
			Total	C	O			
3	A	1	4	2	2		0	0
			Total	C	O			
3	A	1	4	2	2		0	0
			Total	C	O			
3	B	1	4	2	2		0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	D	1	4	2	2	0	0
3	D	1	4	2	2	0	0
3	D	1	4	2	2	0	0
3	D	1	4	2	2	0	0
3	D	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	E	1	4	2	2	0	0

Continued on next page...

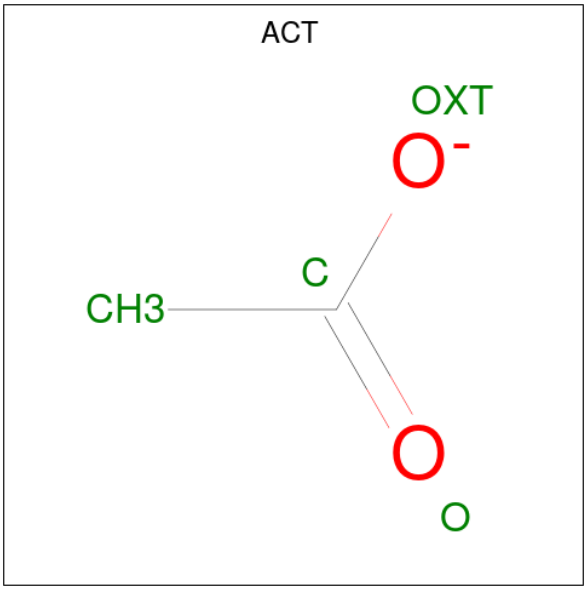
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



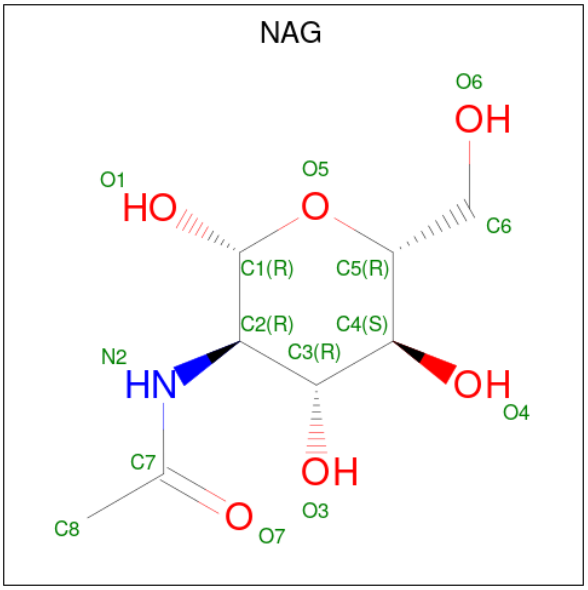
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	B	1	4	2	2		0	0
			Total	C	O			
5	C	1	4	2	2		0	0
			Total	C	O			
5	C	1	4	2	2		0	0
			Total	C	O			
5	D	1	4	2	2		0	0
			Total	C	O			
5	E	1	4	2	2		0	0
			Total	C	O			
5	E	1	4	2	2		0	0
			Total	C	O			
5	E	1	4	2	2		0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	14	8	1	5	0	0
			Total	C	N	O		
6	C	1	14	8	1	5	0	0
			Total	C	N	O		
6	D	1	14	8	1	5	0	0
			Total	C	N	O		
6	E	1	14	8	1	5	0	0

- Molecule 7 is water.

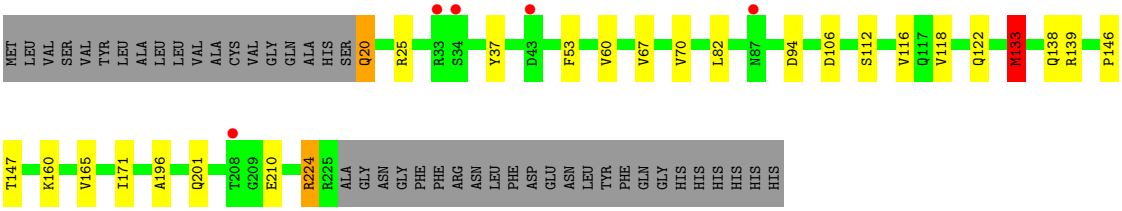
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	173	173	173	0	0
			Total	O		
7	B	135	135	135	0	0
			Total	O		
7	C	136	136	136	0	0
			Total	O		
7	D	134	134	134	0	0
			Total	O		
7	E	171	171	171	0	0

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.

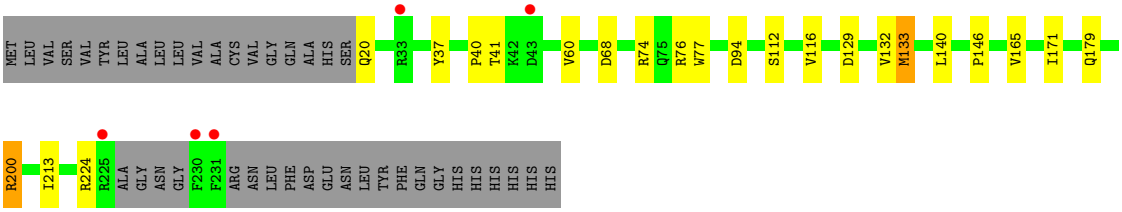
- Molecule 1: Soluble acetylcholine receptor

Chain A:



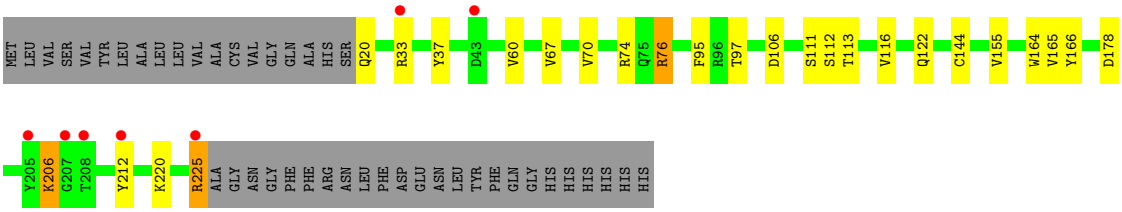
- Molecule 1: Soluble acetylcholine receptor

Chain B:



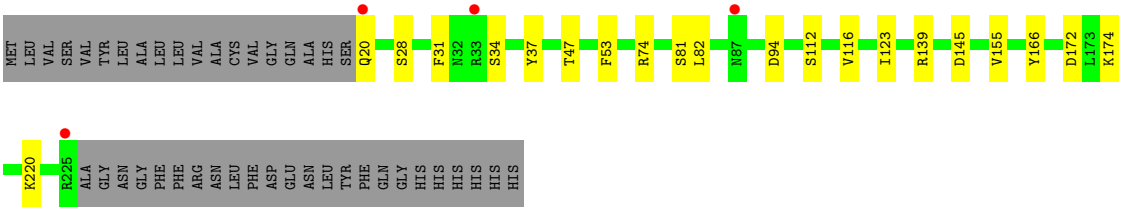
- Molecule 1: Soluble acetylcholine receptor

Chain C:



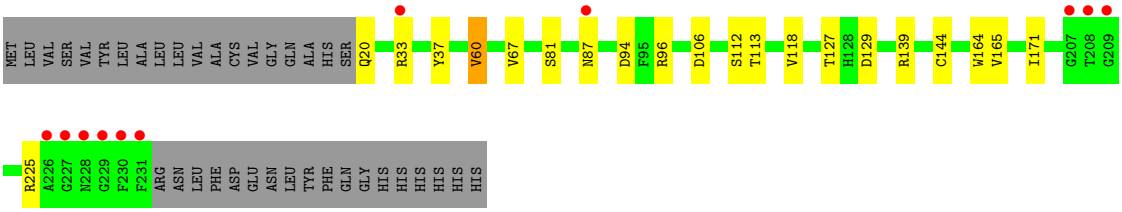
- Molecule 1: Soluble acetylcholine receptor

Chain D:



- Molecule 1: Soluble acetylcholine receptor

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.35Å 100.04Å 163.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 2.00 47.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.92-2.00) 100.0 (47.92-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.197 , 0.250 0.204 , 0.257	Depositor DCC
R_{free} test set	5157 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9478	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ACT, SY9, EDO, NAG

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	0.89	0/1707	0.93	1/2323 (0.0%)
1	B	0.88	0/1725	0.96	5/2346 (0.2%)
1	C	0.85	0/1722	0.95	2/2343 (0.1%)
1	D	0.88	0/1687	0.97	2/2297 (0.1%)
1	E	0.95	0/1761	0.96	2/2395 (0.1%)
All	All	0.89	0/8602	0.96	12/11704 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	145	ASP	CB-CG-OD1	6.68	124.31	118.30
1	C	76[A]	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	C	76[B]	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	A	133	MET	CB-CG-SD	5.60	129.19	112.40
1	E	139	ARG	NE-CZ-NH1	5.54	123.07	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1661	0	1604	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1675	0	1609	14	0
1	C	1672	0	1617	26	0
1	D	1648	0	1586	15	0
1	E	1702	0	1628	15	0
2	A	25	0	22	1	0
2	B	25	0	22	1	0
2	C	50	0	44	12	0
2	D	25	0	22	0	0
2	E	25	0	22	2	0
3	A	28	0	42	8	0
3	B	24	0	36	8	0
3	C	24	0	36	9	0
3	D	20	0	30	8	0
3	E	28	0	41	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	8	0	6	3	0
5	B	4	0	3	2	0
5	C	8	0	6	10	0
5	D	4	0	3	0	0
5	E	12	0	9	4	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	D	14	0	13	0	0
6	E	14	0	13	0	0
7	A	173	0	0	8	1
7	B	135	0	0	1	0
7	C	136	0	0	11	0
7	D	134	0	0	2	0
7	E	171	0	0	4	0
All	All	9478	0	8440	112	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 112 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:E:112:SER:O	5:E:602:ACT:H1	1.72	0.89
1:C:122:GLN:HG3	7:C:830:HOH:O	1.73	0.87
2:C:601[B]:SY9:CAF	7:C:701:HOH:O	2.17	0.87
1:B:112:SER:O	5:B:608:ACT:H1	1.75	0.86
1:B:20:GLN:N	1:B:20:GLN:OE1	2.13	0.81

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:712:HOH:O	7:A:712:HOH:O[2_565]	0.96	1.24

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	206/249 (83%)	203 (98%)	3 (2%)	0	100	100
1	B	206/249 (83%)	200 (97%)	6 (3%)	0	100	100
1	C	207/249 (83%)	201 (97%)	6 (3%)	0	100	100
1	D	204/249 (82%)	202 (99%)	2 (1%)	0	100	100
1	E	213/249 (86%)	209 (98%)	4 (2%)	0	100	100
All	All	1036/1245 (83%)	1015 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	189/222 (85%)	184 (97%)	5 (3%)	46	48
1	B	191/222 (86%)	187 (98%)	4 (2%)	53	57
1	C	190/222 (86%)	183 (96%)	7 (4%)	34	32
1	D	187/222 (84%)	184 (98%)	3 (2%)	62	67
1	E	193/222 (87%)	186 (96%)	7 (4%)	35	34
All	All	950/1110 (86%)	924 (97%)	26 (3%)	46	46

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	206	LYS
1	D	34	SER
1	E	171	ILE
1	D	28	SER
1	D	94	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	201	GLN
1	E	20	GLN
1	E	55	GLN
1	E	32	ASN
1	C	87	ASN

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)

Of 55 ligands modelled in this entry, 5 are monoatomic - leaving 50 for Mogul analysis.

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	EDO	C	606	-	3,3,3	0.76	0	2,2,2	0.57	0
3	EDO	A	608	4	3,3,3	0.37	0	2,2,2	0.60	0
3	EDO	E	610	-	3,3,3	0.33	0	2,2,2	0.83	0
3	EDO	C	611	4	3,3,3	0.99	0	2,2,2	1.33	0
3	EDO	E	603	-	3,3,3	0.66	0	2,2,2	0.17	0
3	EDO	E	609	-	3,3,3	0.78	0	2,2,2	0.27	0
6	NAG	C	604	1	14,14,15	0.59	0	17,19,21	1.75	4 (23%)
5	ACT	E	607	-	3,3,3	0.63	0	3,3,3	0.91	0
2	SY9	E	601	-	31,31,31	0.40	0	51,51,51	0.44	0
3	EDO	C	605	-	3,3,3	0.49	0	2,2,2	0.29	0
3	EDO	D	606	-	3,3,3	0.96	0	2,2,2	1.48	0
3	EDO	D	607	-	3,3,3	0.41	0	2,2,2	0.75	0
3	EDO	A	604	-	3,3,3	0.57	0	2,2,2	0.37	0
3	EDO	E	608	4	3,3,3	1.14	0	2,2,2	1.33	0
3	EDO	B	609	4	3,3,3	1.14	0	2,2,2	1.53	0
3	EDO	C	608	-	3,3,3	0.89	0	2,2,2	0.76	0
3	EDO	B	604	-	3,3,3	0.80	0	2,2,2	1.20	0
5	ACT	C	603	-	3,3,3	1.33	1 (33%)	3,3,3	1.75	2 (66%)
3	EDO	D	605	-	3,3,3	0.82	0	2,2,2	0.77	0
2	SY9	D	601	-	31,31,31	0.34	0	51,51,51	0.39	0
3	EDO	A	602	4	3,3,3	1.13	0	2,2,2	1.29	0
5	ACT	E	602	4	3,3,3	1.15	0	3,3,3	0.92	0
5	ACT	C	610	4	3,3,3	0.80	0	3,3,3	0.52	0
3	EDO	E	611	-	3,3,3	0.38	0	2,2,2	0.84	0
5	ACT	A	610	-	3,3,3	0.88	0	3,3,3	2.46	2 (66%)
2	SY9	C	601[A]	-	31,31,31	0.29	0	51,51,51	0.50	0
6	NAG	B	602	1	14,14,15	0.90	0	17,19,21	3.37	8 (47%)
2	SY9	C	601[B]	-	31,31,31	0.26	0	51,51,51	0.46	0
3	EDO	E	612	-	3,3,3	0.99	0	2,2,2	0.81	0
6	NAG	E	605	1	14,14,15	0.63	0	17,19,21	2.11	6 (35%)
3	EDO	B	605	-	3,3,3	0.50	0	2,2,2	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ACT	E	606	4	3,3,3	1.45	1 (33%)	3,3,3	1.33	0
3	EDO	D	604	-	3,3,3	0.94	0	2,2,2	0.91	0
3	EDO	C	607	-	3,3,3	0.46	0	2,2,2	0.15	0
3	EDO	A	609	-	3,3,3	1.06	0	2,2,2	1.42	0
3	EDO	A	603	-	3,3,3	1.07	0	2,2,2	1.84	1 (50%)
3	EDO	B	610	-	3,3,3	1.20	0	2,2,2	2.04	1 (50%)
3	EDO	A	605	-	3,3,3	0.81	0	2,2,2	1.08	0
3	EDO	B	603	-	3,3,3	0.69	0	2,2,2	0.20	0
5	ACT	D	603	-	3,3,3	0.94	0	3,3,3	0.78	0
2	SY9	A	601	-	31,31,31	0.44	0	51,51,51	0.66	0
3	EDO	A	611	-	3,3,3	0.37	0	2,2,2	0.26	0
3	EDO	E	613	-	3,3,3	1.41	0	2,2,2	0.57	0
3	EDO	C	602	-	3,3,3	0.51	0	2,2,2	1.04	0
3	EDO	B	606	-	3,3,3	0.34	0	2,2,2	0.41	0
2	SY9	B	601	-	31,31,31	0.31	0	51,51,51	0.41	0
3	EDO	D	608	-	3,3,3	0.72	0	2,2,2	1.21	0
5	ACT	A	607	4	3,3,3	1.03	0	3,3,3	0.94	0
6	NAG	D	602	1	14,14,15	0.78	0	17,19,21	2.28	8 (47%)
5	ACT	B	608	4	3,3,3	1.08	0	3,3,3	0.68	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
3	EDO	C	606	-	-	0/1/1/1	-
3	EDO	A	608	4	-	1/1/1/1	-
3	EDO	E	610	-	-	1/1/1/1	-
3	EDO	C	611	4	-	1/1/1/1	-
3	EDO	E	603	-	-	1/1/1/1	-
3	EDO	E	609	-	-	0/1/1/1	-
6	NAG	C	604	1	-	1/6/23/26	0/1/1/1
3	EDO	C	605	-	-	1/1/1/1	-
3	EDO	D	606	-	-	0/1/1/1	-
3	EDO	D	607	-	-	0/1/1/1	-
3	EDO	A	604	-	-	1/1/1/1	-
3	EDO	E	608	4	-	1/1/1/1	-
3	EDO	B	609	4	-	1/1/1/1	-
3	EDO	C	608	-	-	1/1/1/1	-
3	EDO	B	604	-	-	1/1/1/1	-
3	EDO	D	605	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	602	4	-	1/1/1/1	-
3	EDO	E	611	-	-	1/1/1/1	-
6	NAG	B	602	1	-	5/6/23/26	0/1/1/1
3	EDO	E	612	-	-	1/1/1/1	-
6	NAG	E	605	1	-	2/6/23/26	0/1/1/1
3	EDO	B	605	-	-	1/1/1/1	-
3	EDO	D	604	-	-	1/1/1/1	-
3	EDO	C	607	-	-	0/1/1/1	-
3	EDO	A	609	-	-	1/1/1/1	-
3	EDO	A	603	-	-	1/1/1/1	-
3	EDO	B	610	-	-	1/1/1/1	-
3	EDO	A	605	-	-	1/1/1/1	-
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	E	613	-	-	1/1/1/1	-
3	EDO	A	611	-	-	1/1/1/1	-
3	EDO	C	602	-	-	0/1/1/1	-
3	EDO	B	606	-	-	0/1/1/1	-
3	EDO	D	608	-	-	1/1/1/1	-
6	NAG	D	602	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	606	ACT	O-C	2.36	1.33	1.22
5	C	603	ACT	O-C	2.31	1.32	1.22

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	602	NAG	C2-N2-C7	7.63	133.76	122.90
6	B	602	NAG	C8-C7-N2	5.54	125.48	116.10
6	B	602	NAG	C1-C2-N2	-5.12	101.74	110.49
6	D	602	NAG	C4-C3-C2	4.64	117.82	111.02
6	B	602	NAG	O5-C5-C6	4.56	114.35	107.20

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	602	NAG	C3-C2-N2-C7
6	B	602	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	602	NAG	C4-C5-C6-O6
6	B	602	NAG	C8-C7-N2-C2
6	B	602	NAG	O7-C7-N2-C2

There are no ring outliers.

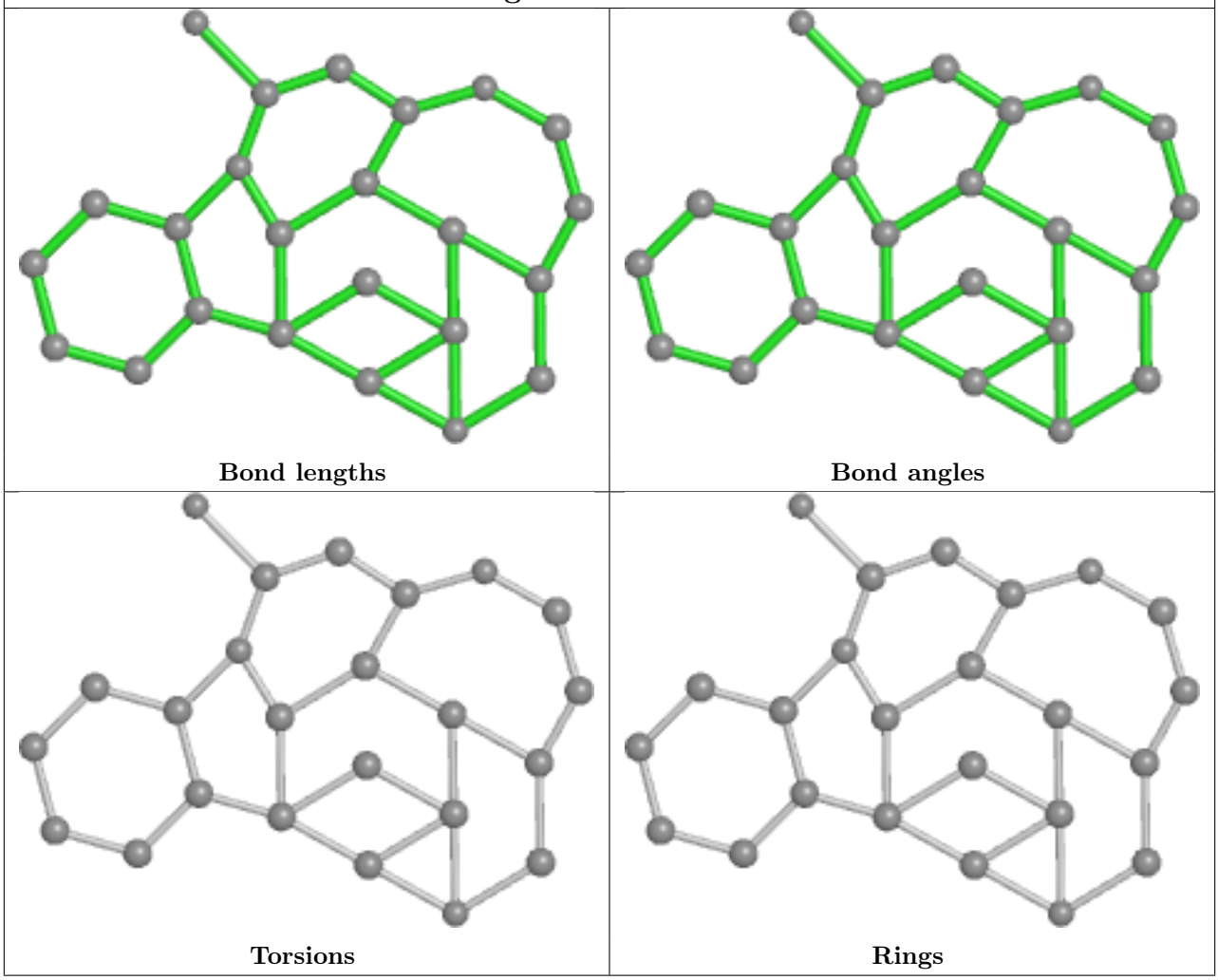
29 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	606	EDO	2	0
3	A	608	EDO	2	0
3	E	610	EDO	1	0
3	C	611	EDO	2	0
2	E	601	SY9	2	0
3	D	606	EDO	1	0
3	E	608	EDO	2	0
3	B	609	EDO	1	0
3	B	604	EDO	2	0
5	C	603	ACT	7	0
3	D	605	EDO	3	0
5	E	602	ACT	3	0
5	C	610	ACT	3	0
5	A	610	ACT	2	0
2	C	601[B]	SY9	12	0
3	B	605	EDO	1	0
5	E	606	ACT	1	0
3	D	604	EDO	3	0
3	A	603	EDO	3	0
3	B	610	EDO	4	0
3	A	605	EDO	1	0
2	A	601	SY9	1	0
3	A	611	EDO	2	0
3	E	613	EDO	1	0
3	C	602	EDO	5	0
2	B	601	SY9	1	0
3	D	608	EDO	1	0
5	A	607	ACT	1	0
5	B	608	ACT	2	0

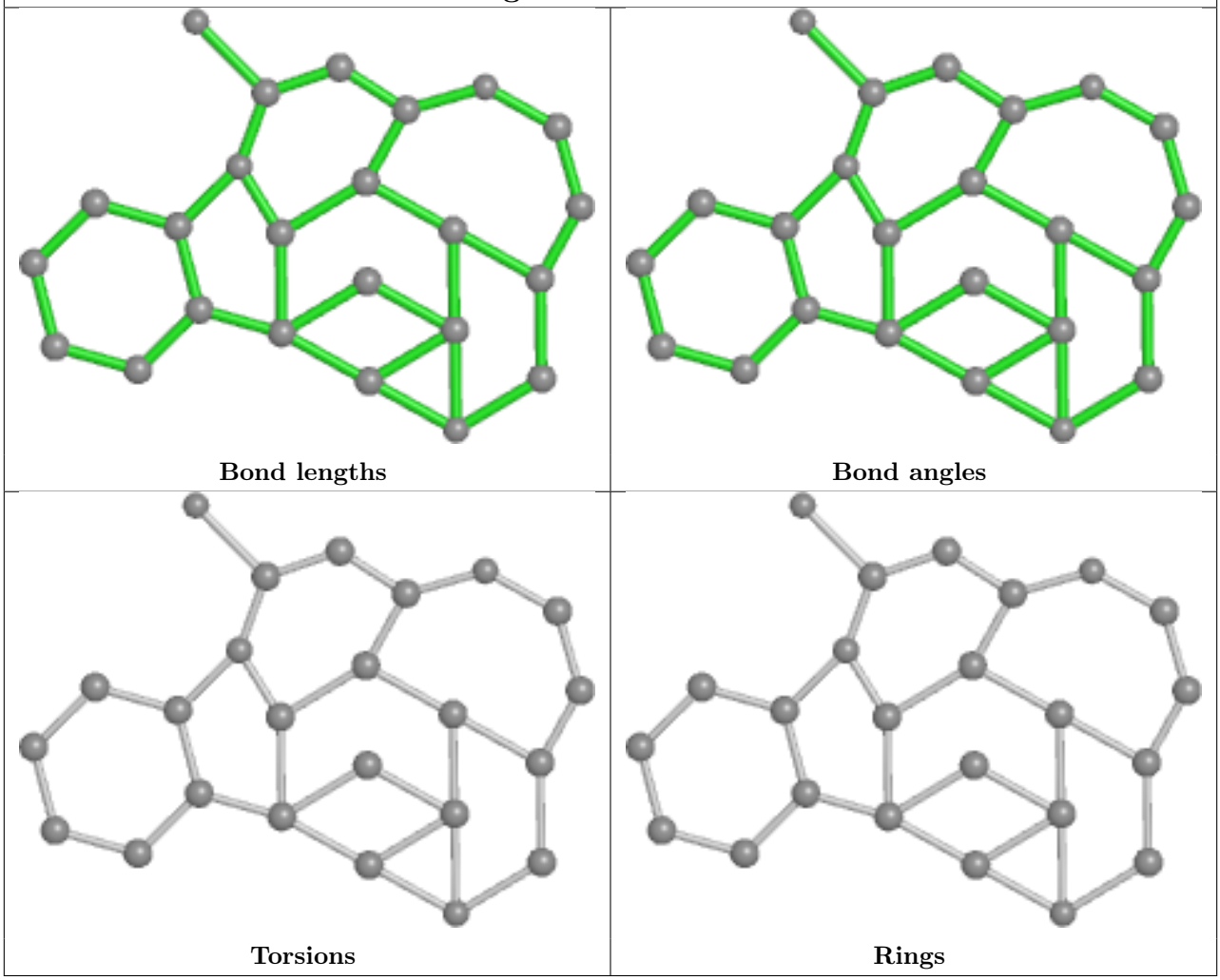
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

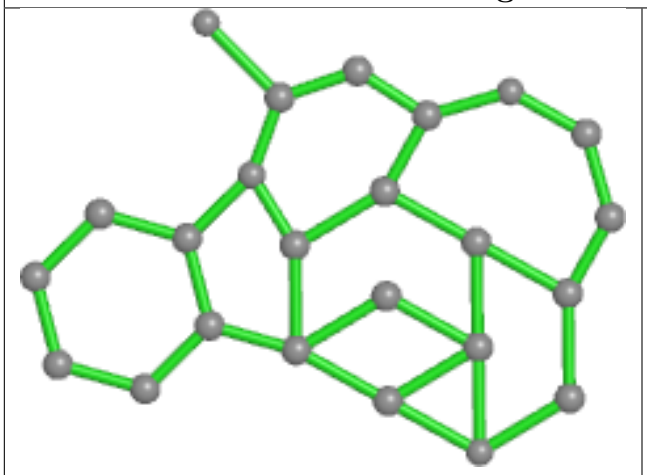
Ligand SY9 E 601



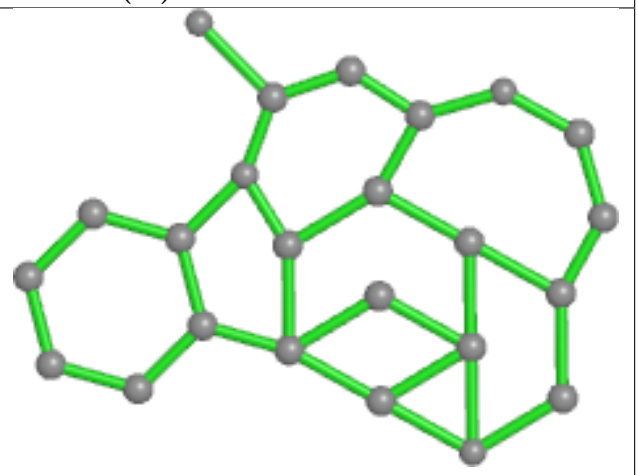
Ligand SY9 D 601



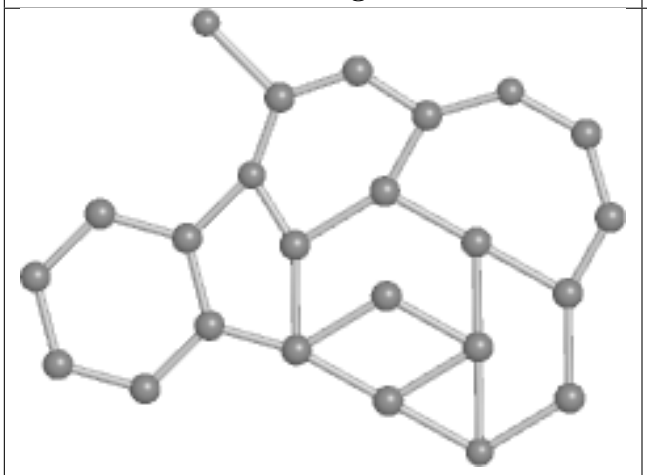
Ligand SY9 C 601 (A)



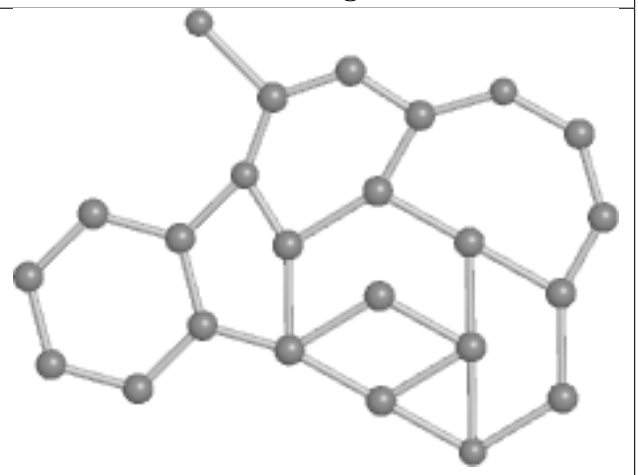
Bond lengths



Bond angles

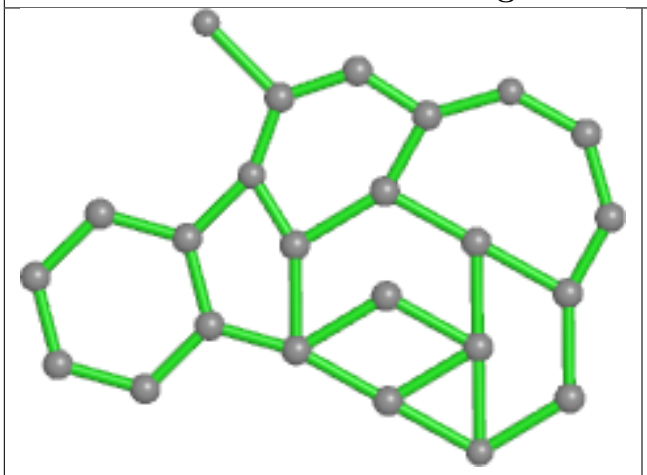


Torsions

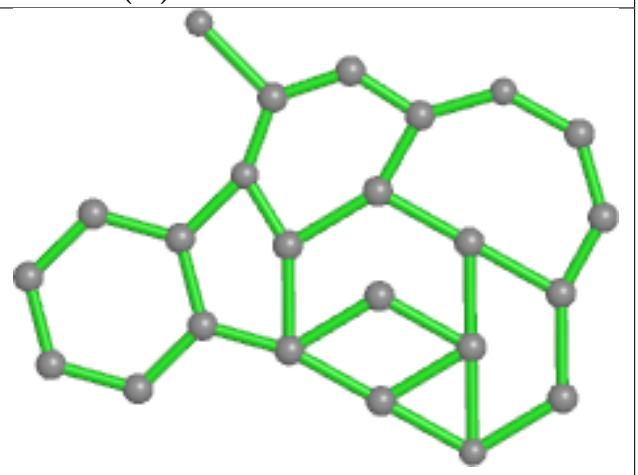


Rings

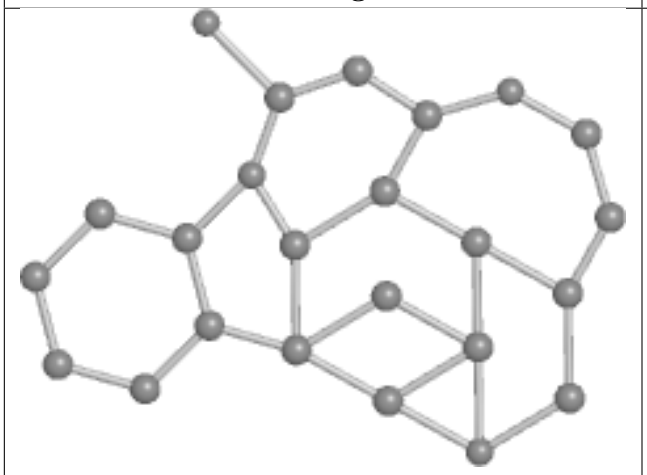
Ligand SY9 C 601 (B)



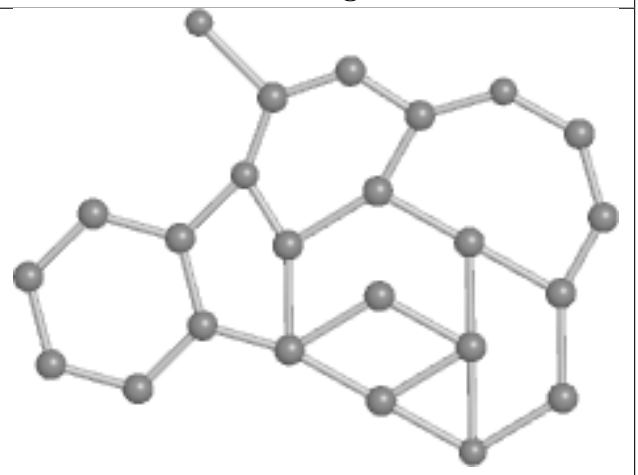
Bond lengths



Bond angles

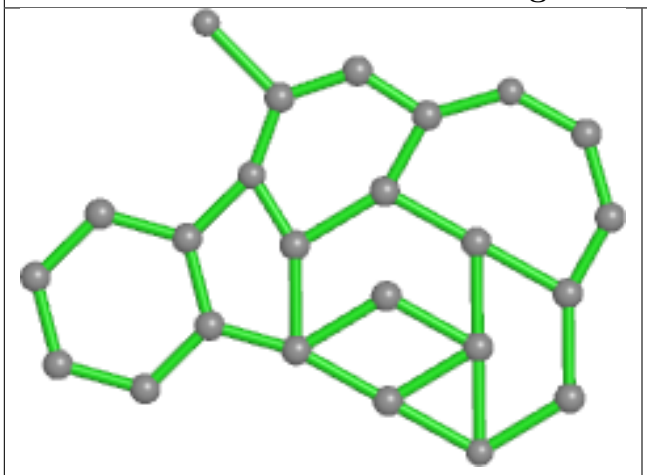


Torsions

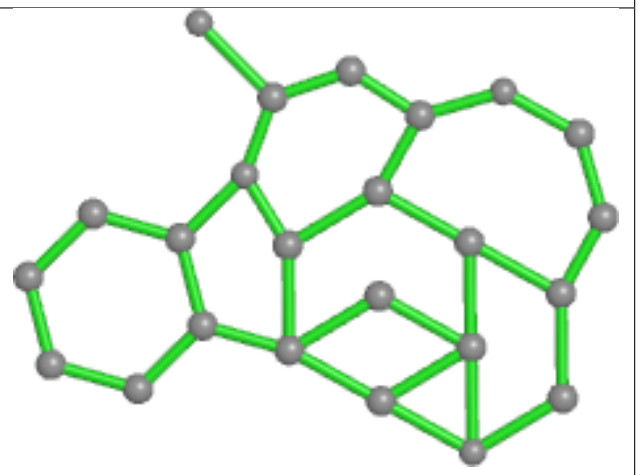


Rings

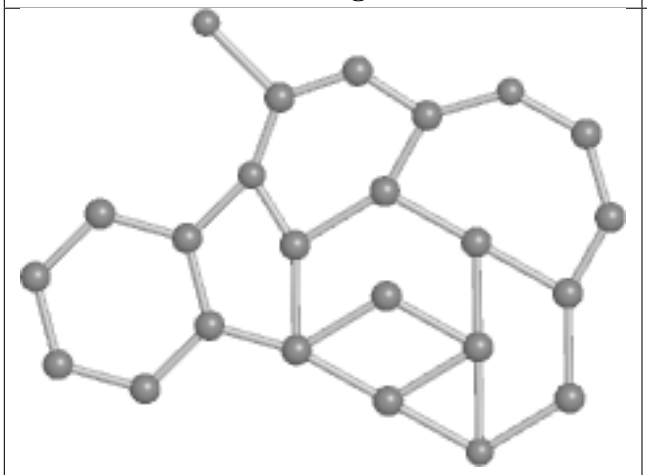
Ligand SY9 A 601



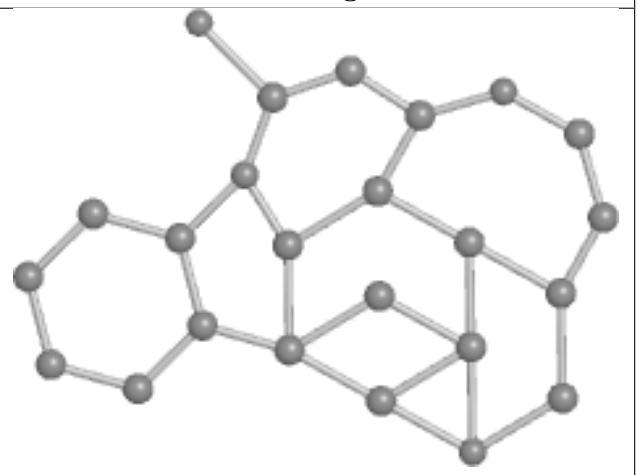
Bond lengths



Bond angles

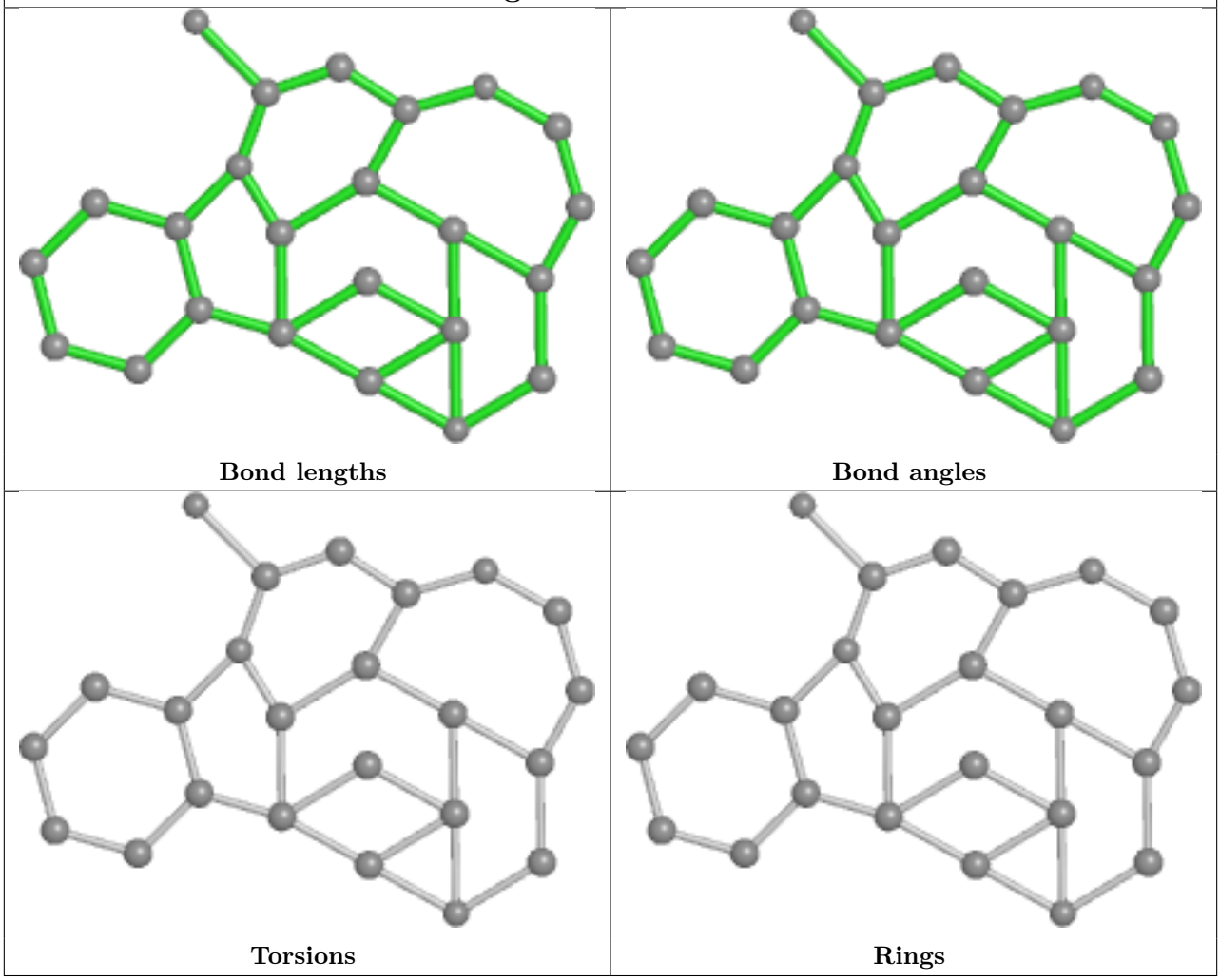


Torsions



Rings

Ligand SY9 B 601



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	206/249 (82%)	-0.02	5 (2%)	59	57	13, 23, 47, 61	0
1	B	208/249 (83%)	-0.02	5 (2%)	59	57	15, 25, 45, 98	0
1	C	206/249 (82%)	0.02	7 (3%)	45	44	17, 25, 49, 95	0
1	D	206/249 (82%)	-0.13	4 (1%)	66	65	15, 24, 42, 70	0
1	E	212/249 (85%)	0.04	11 (5%)	27	26	14, 23, 50, 78	0
All	All	1038/1245 (83%)	-0.02	32 (3%)	49	48	13, 24, 48, 98	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	207	GLY	8.2
1	B	231	PHE	7.5
1	E	226	ALA	6.0
1	E	228	ASN	5.5
1	E	229	GLY	4.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
6	NAG	D	602	14/15	0.50	0.44	79,85,90,92	0
6	NAG	E	605	14/15	0.50	0.48	69,92,106,116	0
6	NAG	B	602	14/15	0.58	0.59	77,97,108,114	0
3	EDO	A	609	4/4	0.63	0.34	46,47,48,51	0
6	NAG	C	604	14/15	0.65	0.56	84,94,104,107	0
3	EDO	D	608	4/4	0.67	0.32	50,51,54,60	0
3	EDO	D	607	4/4	0.77	0.20	38,41,41,43	0
2	SY9	C	601[B]	25/25	0.77	0.25	29,32,33,34	25
2	SY9	C	601[A]	25/25	0.77	0.25	56,61,66,68	25
3	EDO	B	610	4/4	0.80	0.29	37,38,41,42	0
3	EDO	C	611	4/4	0.80	0.20	27,27,28,36	0
3	EDO	B	603	4/4	0.82	0.24	42,44,48,54	0
3	EDO	D	606	4/4	0.82	0.32	45,46,47,47	0
2	SY9	E	601	25/25	0.84	0.15	30,34,40,45	0
3	EDO	E	613	4/4	0.84	0.31	23,24,31,35	0
3	EDO	E	612	4/4	0.85	0.21	27,30,35,37	0
2	SY9	A	601	25/25	0.85	0.14	35,40,47,51	0
3	EDO	E	603	4/4	0.85	0.19	35,39,41,43	0
3	EDO	C	606	4/4	0.86	0.24	20,26,33,34	0
3	EDO	C	602	4/4	0.87	0.24	38,41,44,45	0
3	EDO	D	605	4/4	0.87	0.24	29,31,39,42	0
3	EDO	B	605	4/4	0.87	0.37	41,45,47,52	0
3	EDO	C	607	4/4	0.88	0.30	44,49,50,50	0
3	EDO	C	608	4/4	0.88	0.22	39,42,46,48	0
3	EDO	E	611	4/4	0.88	0.32	40,45,47,49	0
3	EDO	B	604	4/4	0.89	0.22	21,22,32,32	0
3	EDO	A	605	4/4	0.89	0.18	26,27,30,32	0
5	ACT	D	603	4/4	0.89	0.15	31,36,42,43	0
3	EDO	B	609	4/4	0.89	0.23	22,27,28,32	0
2	SY9	B	601	25/25	0.89	0.15	25,31,35,37	0
3	EDO	E	610	4/4	0.89	0.21	36,37,37,45	0
3	EDO	A	604	4/4	0.89	0.17	38,40,42,54	0
3	EDO	A	603	4/4	0.90	0.21	21,23,29,30	0
3	EDO	A	602	4/4	0.90	0.23	21,24,26,32	0
3	EDO	D	604	4/4	0.90	0.17	23,25,36,36	0
5	ACT	A	610	4/4	0.90	0.15	24,27,28,31	0
5	ACT	C	603	4/4	0.90	0.13	23,25,27,29	0
3	EDO	B	606	4/4	0.91	0.41	53,53,55,60	0
5	ACT	E	607	4/4	0.91	0.21	43,48,51,54	0
5	ACT	C	610	4/4	0.91	0.14	18,19,23,26	0
3	EDO	C	605	4/4	0.92	0.14	36,42,44,52	0

Continued on next page...

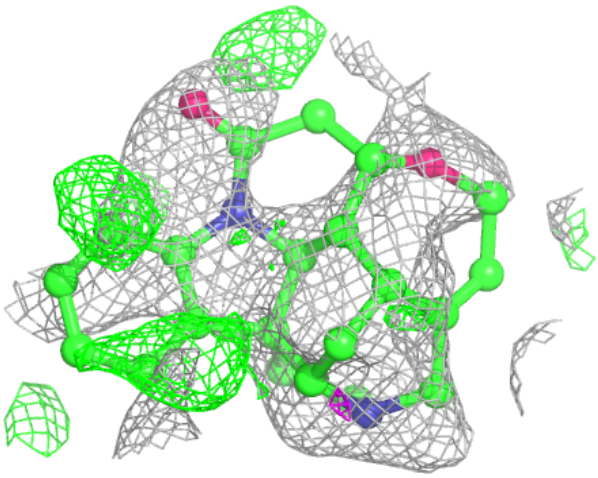
Continued from previous page...

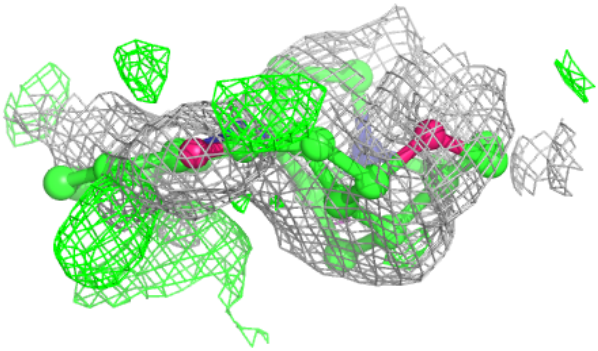
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	B	608	4/4	0.92	0.15	16,17,18,21	0
3	EDO	E	609	4/4	0.93	0.18	30,36,44,51	0
2	SY9	D	601	25/25	0.93	0.12	22,25,31,33	0
3	EDO	E	608	4/4	0.93	0.18	23,27,29,35	0
5	ACT	E	606	4/4	0.94	0.15	15,18,19,19	0
3	EDO	A	611	4/4	0.94	0.20	35,39,41,45	0
5	ACT	E	602	4/4	0.94	0.11	14,16,19,19	0
4	NA	A	606	1/1	0.96	0.11	19,19,19,19	0
4	NA	E	604	1/1	0.96	0.07	23,23,23,23	0
5	ACT	A	607	4/4	0.96	0.10	14,18,19,19	0
3	EDO	A	608	4/4	0.97	0.14	23,23,25,37	0
4	NA	D	609	1/1	0.97	0.11	25,25,25,25	0
4	NA	C	609	1/1	0.98	0.17	27,27,27,27	0
4	NA	B	607	1/1	0.99	0.05	24,24,24,24	0

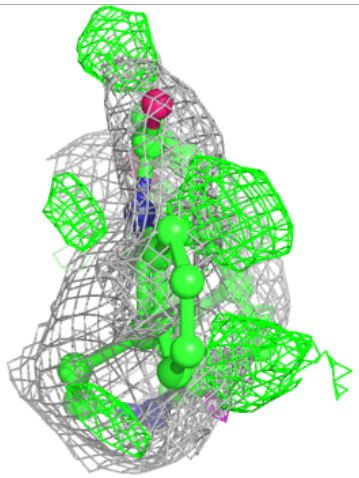
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SY9 C 601 (B):

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

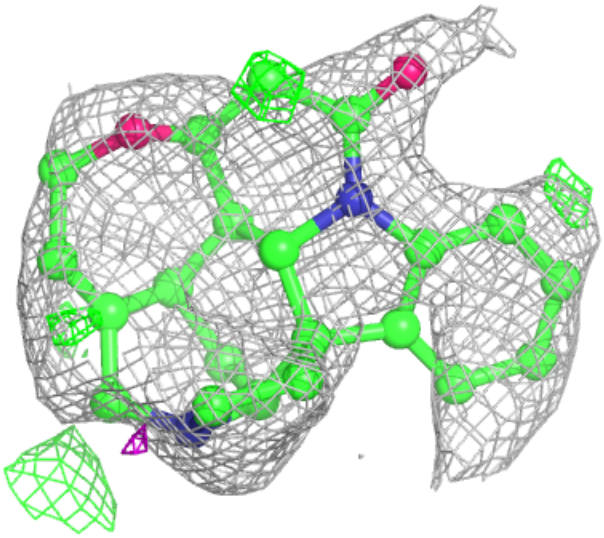


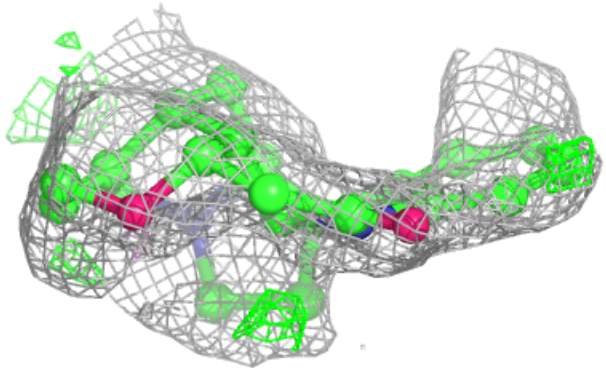


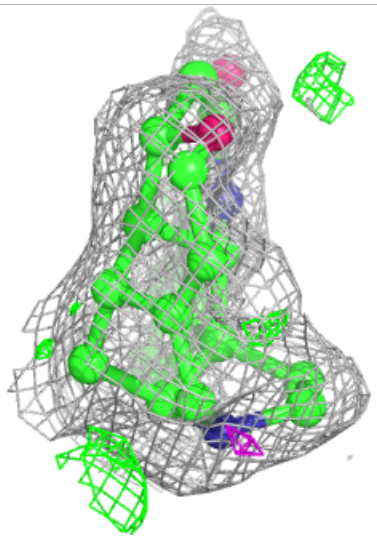


Electron density around SY9 C 601 (A):

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

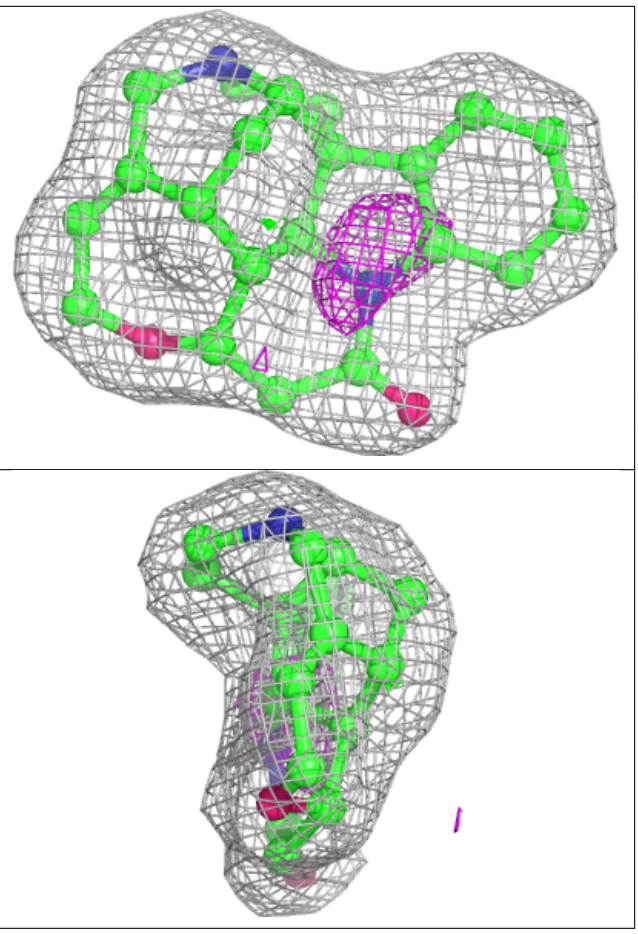


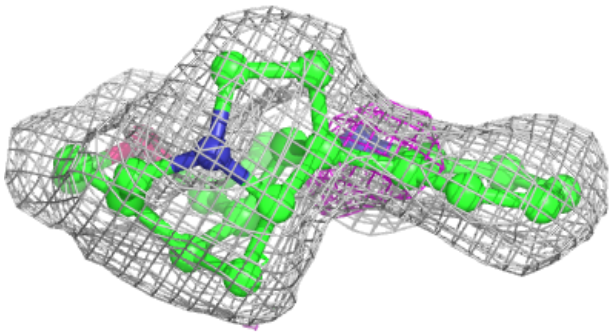




Electron density around SY9 E 601:

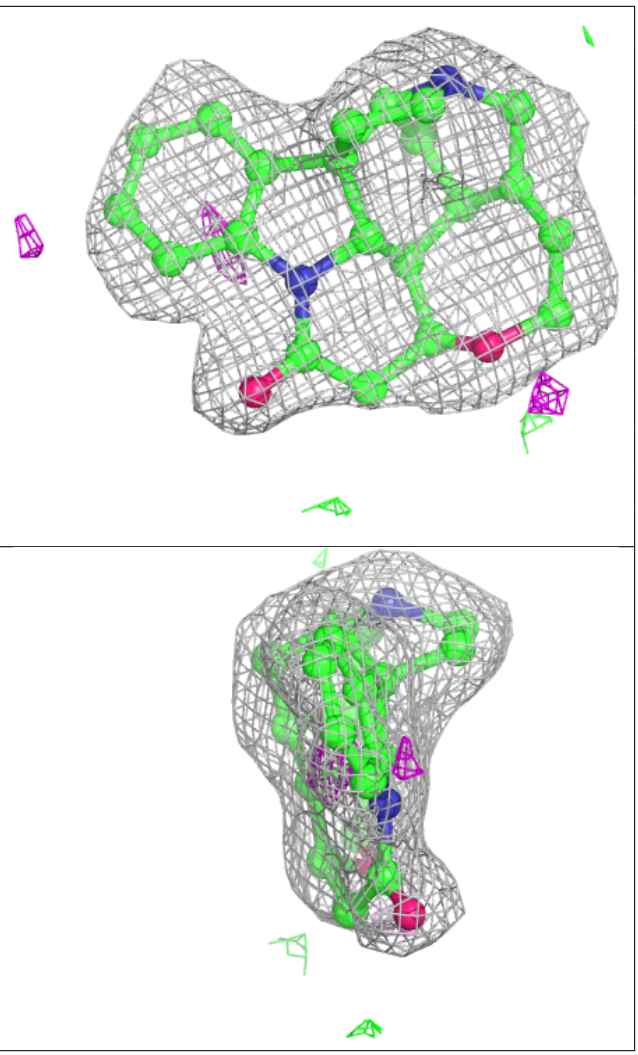
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

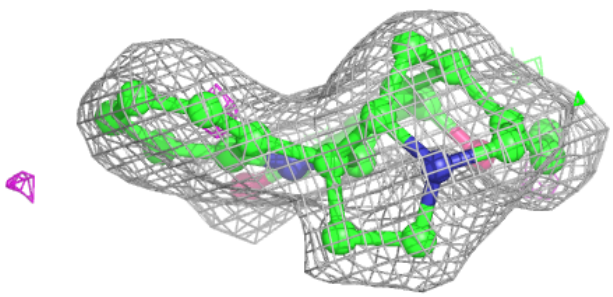




Electron density around SY9 A 601:

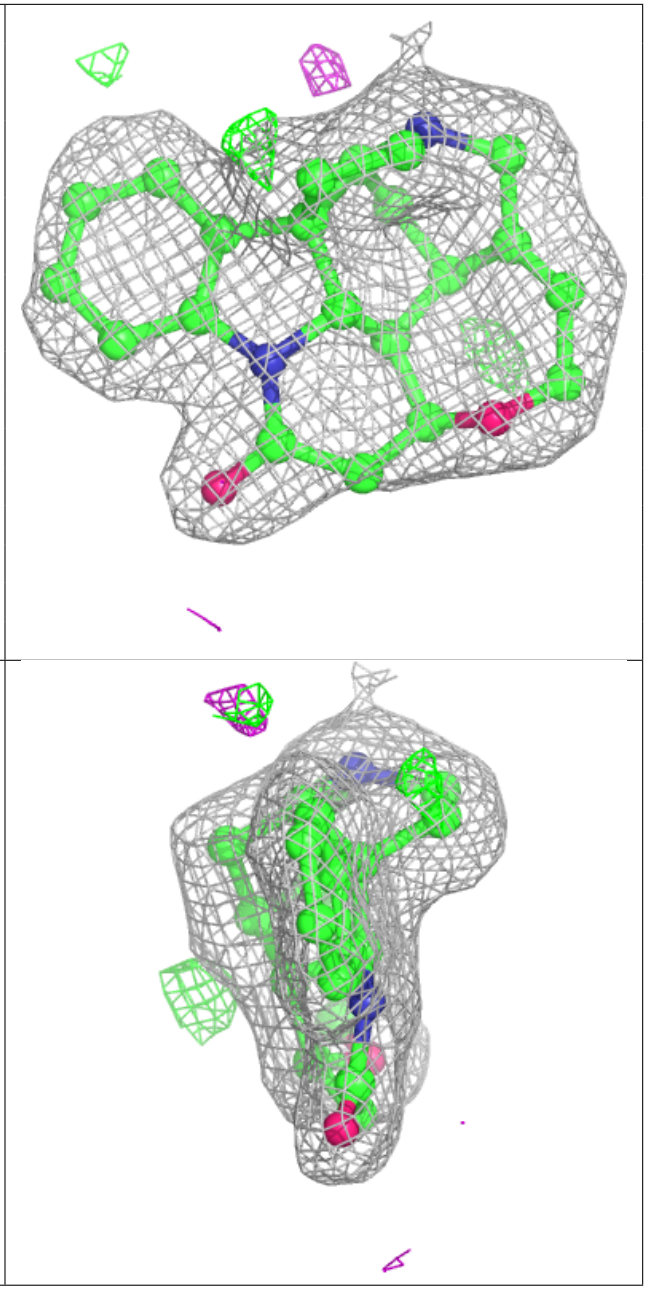
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





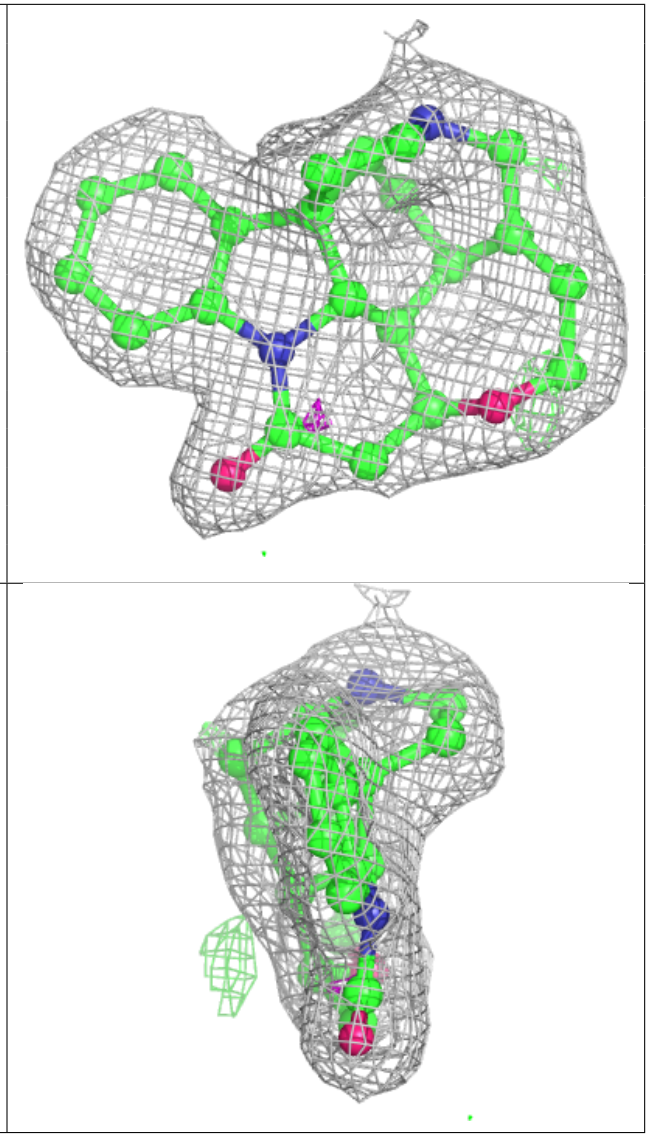
Electron density around SY9 B 601:

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



Electron density around SY9 D 601:

$2mF_o$-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.