Full wwPDB X-ray Structure Validation Report (i)

Apr 18, 2024 – 04:04 pm BST

PDB ID	:	8ORC
Title	:	Mus Musculus Acetylcholinesterase in complex with AL237
Authors	:	Ekstrom, F.E.; Linusson, A.
Deposited on	:	2023-04-13
Resolution	:	2.10 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:

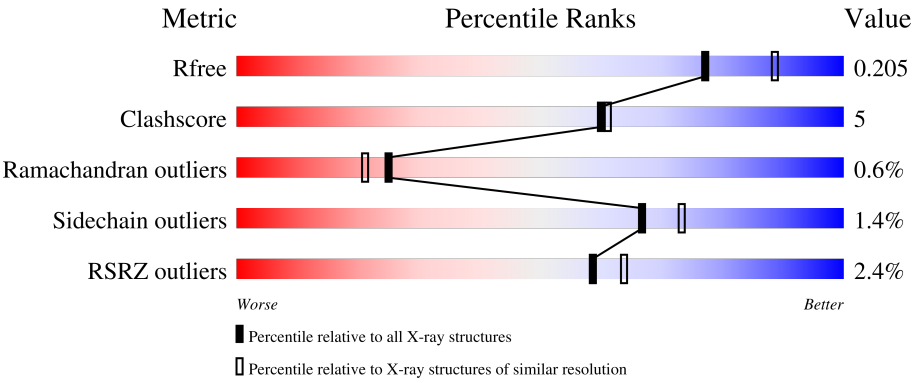
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	543	2% 89% 9%
1	B	543	3% 91% 7%

2 Entry composition

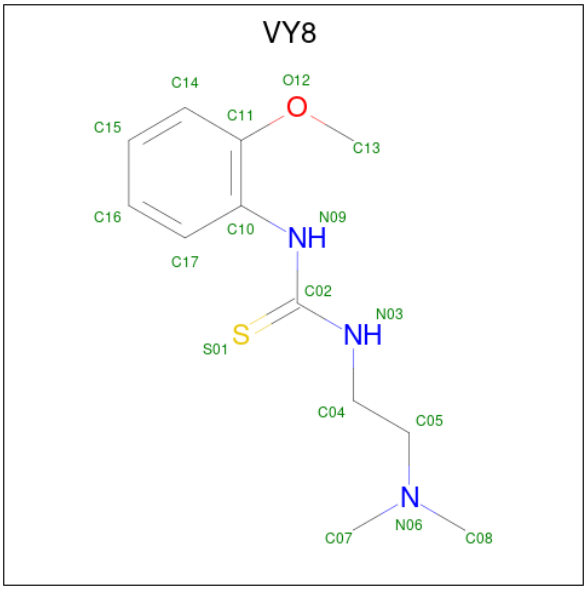
There are 7 unique types of molecules in this entry. The entry contains 17386 atoms, of which 8330 are hydrogens and 0 are deuteriums.

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 Acetylcholinesterase.

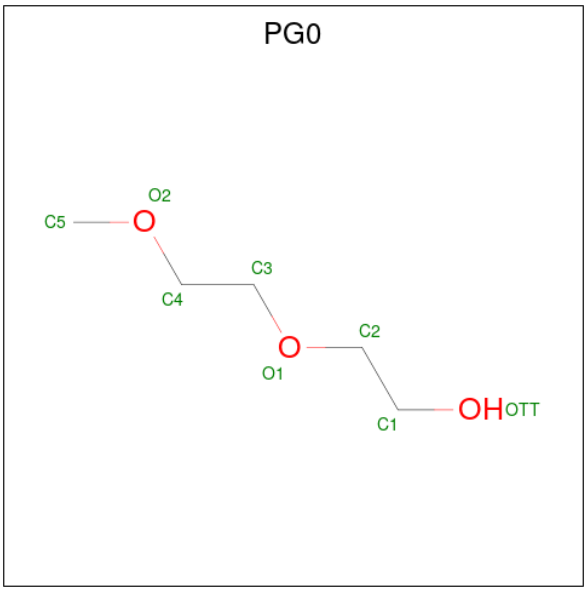
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	536	Total	C	H	N	O	S	0	7	0
			8306	2703	4093	731	765	14			
1	B	534	Total	C	H	N	O	S	7	1	0
			8210	2676	4043	721	756	14			

- Molecule 2 is 1-[2-(dimethylamino)ethyl]-3-(2-methoxyphenyl)thiourea (three-letter code: VY8) (formula: $C_{12}H_{19}N_3OS$) (labeled as "Ligand of Interest" by depositor).



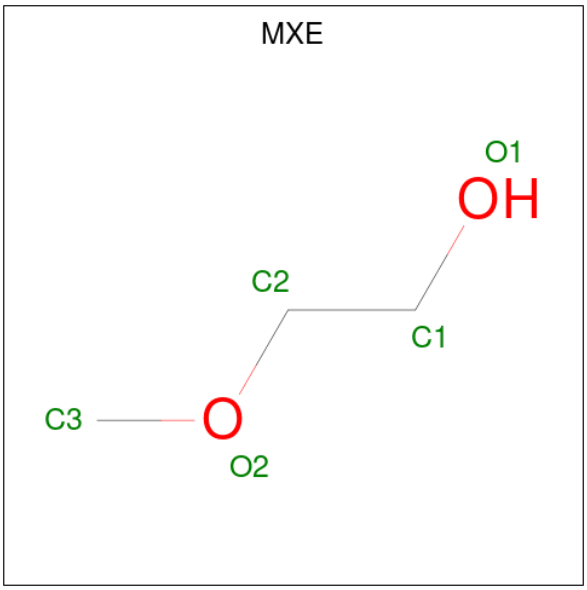
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			36	12	19	3	1	1		
2	B	1	Total	C	H	N	O	S	0	0
			36	12	19	3	1	1		

- Molecule 3 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



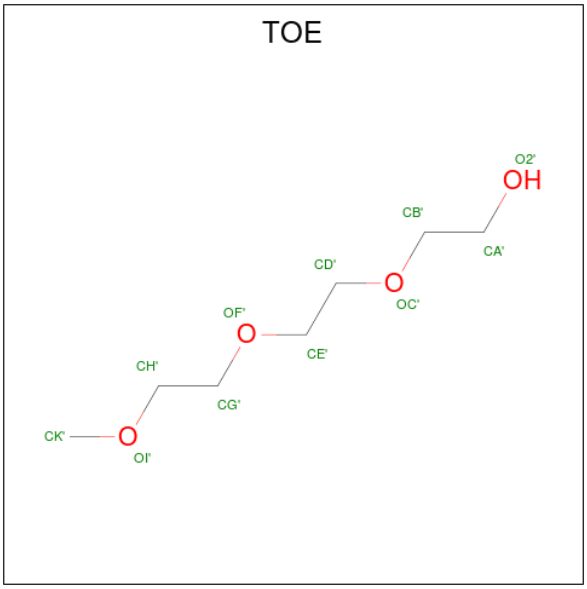
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	B	1	Total	C	H	O	0	0
			20	5	12	3		
3	B	1	Total	C	H	O	0	0
			20	5	12	3		
3	B	1	Total	C	H	O	0	0
			20	5	12	3		

- Molecule 4 is 2-METHOXYETHANOL (three-letter code: MXE) (formula: $C_3H_8O_2$).



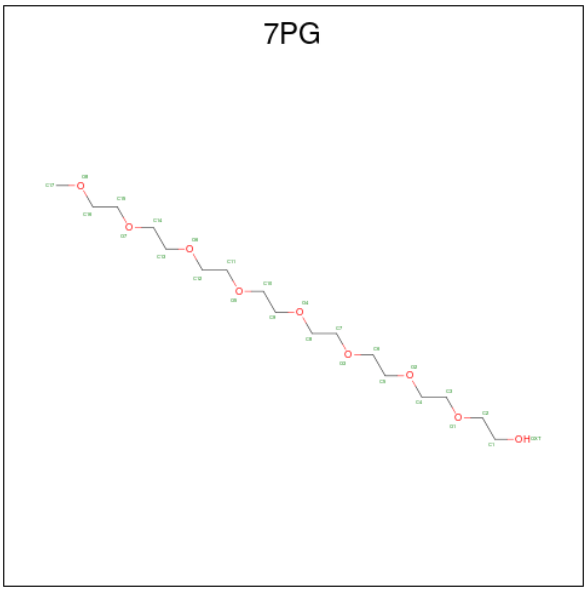
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 13 3 8 2	0	0
4	A	1	Total C H O 13 3 8 2	0	0
4	B	1	Total C H O 13 3 8 2	0	0
4	B	1	Total C H O 13 3 8 2	0	0
4	B	1	Total C H O 13 3 8 2	0	0

- Molecule 5 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (three-letter code: TOE) (formula: $C_7H_{16}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 27 7 16 4	0	0
5	A	1	Total C H O 27 7 16 4	0	0

- Molecule 6 is 2,5,8,11,14,17,20,23-OCTAOXAPENTACOSAN-25-OL (three-letter code: 7PG) (formula: $C_{17}H_{36}O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			62	17	36	9		

- Molecule 7 is water.

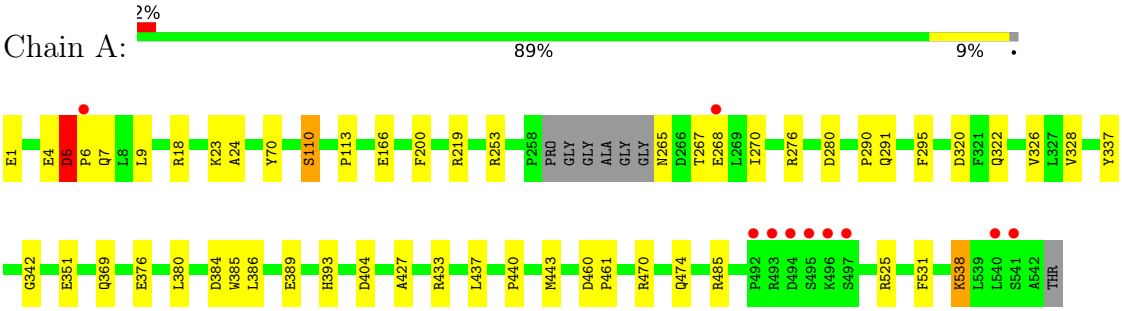
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	294	Total	O	0	0
			294	294		
7	B	243	Total	O	0	0
			243	243		

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.

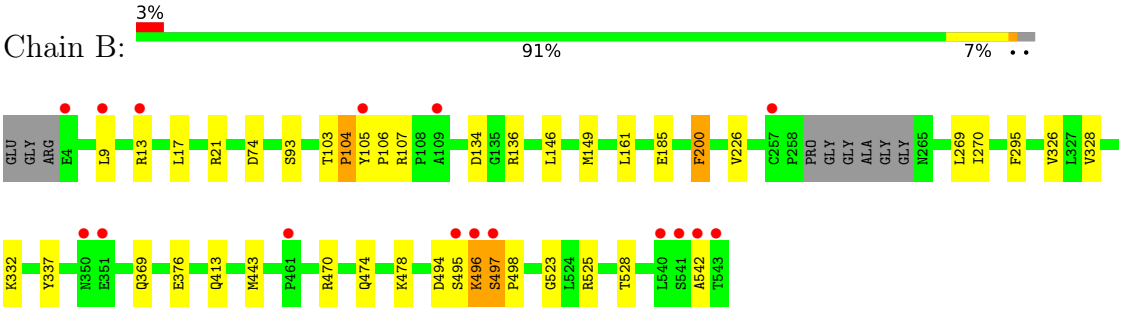
• Molecule 1: Acetylcholinesterase

Chain A:



• Molecule 1: Acetylcholinesterase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.61Å 112.11Å 226.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.23 – 2.10 49.23 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.23-2.10) 99.8 (49.23-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.186 , 0.207 0.185 , 0.205	Depositor DCC
R_{free} test set	2379 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 71.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17386	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: MXE, TOE, VY8, 7PG, PG0

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	0.32	1/4349 (0.0%)	0.54	0/5945
1	B	0.35	2/4291 (0.0%)	0.55	1/5865 (0.0%)
All	All	0.33	3/8640 (0.0%)	0.54	1/11810 (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	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	PRO	N-CA	12.96	1.69	1.47
1	A	290	PRO	N-CD	-8.37	1.36	1.47
1	B	103	THR	C-N	5.65	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	104	PRO	CA-N-CD	-7.67	100.76	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	106	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	B	107	ARG	Mainchain

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	4213	4093	4075	44	1
1	B	4167	4043	4053	36	1
2	A	17	19	0	0	0
2	B	17	19	0	0	0
3	A	8	12	12	0	0
3	B	24	36	36	0	0
4	A	10	16	16	0	0
4	B	15	24	24	0	0
5	A	22	32	32	0	0
6	B	26	36	36	1	0
7	A	294	0	0	10	0
7	B	243	0	0	5	0
All	All	9056	8330	8284	78	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 5.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:PRO:N	1:B:104:PRO:CA	1.69	1.36
1:B:496:LYS:CE	1:B:498:PRO:HB3	1.89	1.02
1:B:369:GLN:N	1:B:369:GLN:OE1	1.99	0.96
1:B:494:ASP:OD1	1:B:495:SER:N	2.07	0.88
1:B:496:LYS:HE3	1:B:498:PRO:HB3	1.56	0.87
1:A:351:GLU:OE2	7:A:701:HOH:O	1.95	0.84
1:B:496:LYS:NZ	1:B:498:PRO:HB3	1.95	0.80
1:A:6:PRO:HB2	7:A:928:HOH:O	1.82	0.79
1:A:531:PHE:HB2	6:B:601:7PG:H72	1.66	0.76
1:A:6:PRO:CG	7:A:928:HOH:O	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLU:OE2	1:A:380:LEU:HD21	1.90	0.70
1:A:276[A]:ARG:NH1	1:A:280:ASP:OD2	2.25	0.70
1:A:265:ASN:OD1	1:A:268:GLU:HG3	1.92	0.69
1:A:6:PRO:CB	7:A:928:HOH:O	2.40	0.69
1:A:389:GLU:OE1	7:A:702:HOH:O	2.10	0.68
1:B:413[A]:GLN:OE1	7:B:701:HOH:O	2.10	0.68
1:A:393:HIS:CD2	7:A:872:HOH:O	2.47	0.68
1:B:496:LYS:HG3	1:B:496:LYS:O	1.94	0.68
1:A:4:GLU:OE2	1:A:18:ARG:HD3	1.96	0.65
1:B:104:PRO:N	1:B:104:PRO:C	2.49	0.65
1:B:332:LYS:HD3	7:B:799:HOH:O	2.01	0.60
1:B:104:PRO:HB3	7:B:843:HOH:O	2.01	0.60
1:B:496:LYS:NZ	7:B:706:HOH:O	2.37	0.58
1:A:538:LYS:HD3	1:B:376:GLU:OE1	2.03	0.57
1:B:497:SER:N	1:B:498:PRO:HA	2.20	0.57
1:A:393:HIS:HD2	7:A:872:HOH:O	1.85	0.56
1:A:5:ASP:HB2	1:A:6:PRO:HA	1.91	0.53
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.92	0.52
1:A:384:ASP:HB2	1:A:393:HIS:CE1	2.45	0.51
1:B:74:ASP:OD2	7:B:702:HOH:O	2.18	0.51
1:A:1:GLU:HA	1:A:1:GLU:OE1	2.09	0.51
1:B:21:ARG:HG3	1:B:105:TYR:CD2	2.46	0.51
1:A:291:GLN:OE1	1:A:369[B]:GLN:NE2	2.44	0.50
1:A:5:ASP:HB3	1:A:7[A]:GLN:H	1.77	0.50
1:B:496:LYS:HD2	1:B:498:PRO:HA	1.94	0.50
1:B:496:LYS:HZ1	1:B:498:PRO:HB3	1.76	0.50
1:A:433:ARG:CZ	1:A:437:LEU:HD23	2.42	0.49
1:A:380:LEU:HD12	1:A:385:TRP:CZ2	2.47	0.49
1:A:1:GLU:HG2	7:A:939:HOH:O	2.13	0.49
1:A:4:GLU:O	1:A:5:ASP:HB2	2.11	0.49
1:B:470:ARG:O	1:B:474:GLN:HG3	2.13	0.48
1:A:6:PRO:HG2	7:A:928:HOH:O	2.08	0.48
1:A:166:GLU:OE1	1:A:267:THR:HG23	2.13	0.48
1:A:253:ARG:HD3	7:A:708:HOH:O	2.13	0.48
1:B:497:SER:N	1:B:498:PRO:CA	2.76	0.47
1:B:496:LYS:HD2	1:B:498:PRO:CB	2.44	0.47
1:B:134:ASP:OD1	1:B:136:ARG:HB2	2.15	0.47
1:B:496:LYS:C	1:B:498:PRO:HA	2.34	0.47
1:A:4:GLU:OE2	1:A:18:ARG:CD	2.62	0.46
1:B:337:TYR:HA	1:B:443:MET:CE	2.45	0.46
1:B:525:ARG:HG2	1:B:528:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:O	1:A:427:ALA:HA	2.16	0.46
1:B:496:LYS:CD	1:B:498:PRO:HB3	2.45	0.45
1:A:320:ASP:OD1	1:A:322:GLN:HG3	2.16	0.45
1:A:404:ASP:OD1	1:A:525:ARG:NH2	2.50	0.45
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.98	0.45
1:A:460:ASP:OD1	1:A:461:PRO:HD2	2.16	0.45
1:A:6:PRO:HB2	1:A:9:LEU:HD12	1.99	0.44
1:A:386:LEU:HD11	1:B:523:GLY:HA3	1.99	0.44
1:A:376:GLU:O	1:A:380:LEU:CD2	2.66	0.43
1:A:440:PRO:HD2	1:A:443:MET:SD	2.59	0.43
1:A:380:LEU:CD1	1:A:385:TRP:CZ2	3.02	0.42
1:A:113:PRO:HG2	1:A:485:ARG:HG2	2.02	0.42
1:A:470:ARG:HH11	1:A:470:ARG:HG2	1.85	0.42
1:B:496:LYS:HD2	1:B:498:PRO:CA	2.49	0.42
1:A:4:GLU:O	1:A:5:ASP:CB	2.68	0.42
1:A:337:TYR:HA	1:A:443:MET:CE	2.50	0.41
1:A:470:ARG:O	1:A:474:GLN:HG3	2.20	0.41
1:B:13:ARG:NH1	1:B:185:GLU:OE1	2.54	0.41
1:B:161:LEU:HD12	1:B:270:ILE:HD11	2.03	0.41
1:B:21:ARG:HD3	1:B:105:TYR:CE2	2.55	0.41
1:B:200:PHE:CB	1:B:226:VAL:HB	2.51	0.41
1:A:166:GLU:HB2	1:A:270:ILE:HD13	2.04	0.40
1:B:496:LYS:NZ	1:B:498:PRO:CB	2.75	0.40
1:B:9:LEU:HD23	1:B:17:LEU:O	2.21	0.40
1:B:326:VAL:HG12	1:B:328:VAL:HG13	2.02	0.40
1:A:23:LYS:HE2	1:A:24:ALA:O	2.22	0.40
1:A:376:GLU:O	1:A:380:LEU:HD22	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLU:OE2	1:B:93:SER:OG[2_555]	1.91	0.29

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	539/543 (99%)	516 (96%)	20 (4%)	3 (1%)	25	21
1	B	531/543 (98%)	510 (96%)	18 (3%)	3 (1%)	25	21
All	All	1070/1086 (98%)	1026 (96%)	38 (4%)	6 (1%)	25	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	B	542	ALA
1	A	110	SER
1	B	496	LYS
1	A	342	GLY
1	B	497	SER

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	441/443 (100%)	434 (98%)	7 (2%)	62	69
1	B	438/443 (99%)	433 (99%)	5 (1%)	73	79
All	All	879/886 (99%)	867 (99%)	12 (1%)	67	73

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

Mol	Chain	Res	Type
1	A	5	ASP
1	A	70	TYR
1	A	110	SER
1	A	200	PHE
1	A	219	ARG
1	A	295	PHE

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Mol	Chain	Res	Type
1	A	538	LYS
1	B	146	LEU
1	B	149	MET
1	B	200	PHE
1	B	295	PHE
1	B	478	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	181	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

14 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	$\#\|Z\| > 2$
4	MXE	B	608	-	4,4,4	0.59	0	3,3,3	0.76	0
5	TOE	A	605	-	10,10,10	0.66	0	9,9,9	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MXE	A	603	-	4,4,4	0.53	0	3,3,3	0.74	0
6	7PG	B	601	-	25,25,25	1.13	0	24,24,24	0.79	0
3	PG0	B	603	-	7,7,7	0.63	0	6,6,6	0.73	0
2	VY8	A	601	-	17,17,17	1.48	2 (11%)	21,21,21	1.24	3 (14%)
5	TOE	A	606	-	10,10,10	0.65	0	9,9,9	0.93	0
3	PG0	B	605	-	7,7,7	0.61	0	6,6,6	0.73	0
3	PG0	A	602	-	7,7,7	0.63	0	6,6,6	0.96	0
4	MXE	B	606	-	4,4,4	0.57	0	3,3,3	0.76	0
2	VY8	B	602	-	17,17,17	1.57	2 (11%)	21,21,21	1.32	3 (14%)
3	PG0	B	604	-	7,7,7	0.64	0	6,6,6	0.74	0
4	MXE	B	607	-	4,4,4	0.63	0	3,3,3	0.73	0
4	MXE	A	604	-	4,4,4	0.60	0	3,3,3	0.74	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
4	MXE	B	608	-	-	0/2/2/2	-
5	TOE	A	605	-	-	5/8/8/8	-
4	MXE	A	603	-	-	0/2/2/2	-
6	7PG	B	601	-	-	12/23/23/23	-
3	PG0	B	603	-	-	3/5/5/5	-
2	VY8	A	601	-	-	3/12/12/12	0/1/1/1
5	TOE	A	606	-	-	7/8/8/8	-
3	PG0	B	605	-	-	5/5/5/5	-
3	PG0	A	602	-	-	2/5/5/5	-
4	MXE	B	606	-	-	1/2/2/2	-
2	VY8	B	602	-	-	2/12/12/12	0/1/1/1
3	PG0	B	604	-	-	4/5/5/5	-
4	MXE	B	607	-	-	1/2/2/2	-
4	MXE	A	604	-	-	1/2/2/2	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	VY8	C02-N03	4.42	1.41	1.33
2	A	601	VY8	C02-N03	4.18	1.40	1.33
2	B	602	VY8	C02-N09	2.40	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	VY8	C02-N09	2.05	1.38	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	VY8	C11-C10-N09	2.70	121.51	116.66
2	B	602	VY8	C11-C10-N09	2.64	121.39	116.66
2	B	602	VY8	O12-C11-C10	2.55	117.93	114.80
2	B	602	VY8	S01-C02-N03	-2.48	119.06	123.22
2	A	601	VY8	S01-C02-N03	-2.29	119.38	123.22
2	A	601	VY8	O12-C11-C10	2.23	117.53	114.80

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	7PG	C7-C8-O4-C9
4	B	606	MXE	O1-C1-C2-O2
6	B	601	7PG	O2-C5-C6-O3
5	A	605	TOE	OF'-CG'-CH'-OI'
3	B	604	PG0	O1-C3-C4-O2
5	A	605	TOE	OC'-CD'-CE'-OF'
6	B	601	7PG	O5-C10-C9-O4
3	B	605	PG0	O1-C3-C4-O2
6	B	601	7PG	OXT-C1-C2-O1
6	B	601	7PG	O5-C11-C12-O6
3	A	602	PG0	O1-C3-C4-O2
3	B	603	PG0	OTT-C1-C2-O1
4	B	607	MXE	O1-C1-C2-O2
5	A	606	TOE	O2'-CA'-CB'-OC'
3	B	605	PG0	OTT-C1-C2-O1
3	A	602	PG0	OTT-C1-C2-O1
6	B	601	7PG	C15-C16-O8-C17
2	A	601	VY8	C04-C05-N06-C08
5	A	605	TOE	CE'-CD'-OC'-CB'
3	B	603	PG0	C4-C3-O1-C2
6	B	601	7PG	C11-C12-O6-C13
5	A	605	TOE	CA'-CB'-OC'-CD'
3	B	605	PG0	C1-C2-O1-C3
3	B	604	PG0	C4-C3-O1-C2
6	B	601	7PG	C1-C2-O1-C3
2	A	601	VY8	C04-C05-N06-C07

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Mol	Chain	Res	Type	Atoms
3	B	605	PG0	C4-C3-O1-C2
2	B	602	VY8	C04-C05-N06-C07
4	A	604	MXE	C1-C2-O2-C3
2	B	602	VY8	C04-C05-N06-C08
5	A	606	TOE	CA'-CB'-OC'-CD'
3	B	605	PG0	C3-C4-O2-C5
5	A	606	TOE	OF'-CG'-CH'-OI'
3	B	603	PG0	O1-C3-C4-O2
6	B	601	7PG	O1-C3-C4-O2
5	A	606	TOE	CH'-CG'-OF'-CE'
6	B	601	7PG	C6-C5-O2-C4
6	B	601	7PG	C4-C3-O1-C2
5	A	606	TOE	OC'-CD'-CE'-OF'
2	A	601	VY8	C11-C10-N09-C02
3	B	604	PG0	C3-C4-O2-C5
5	A	605	TOE	CG'-CH'-OI'-CK'
6	B	601	7PG	C13-C14-O7-C15
5	A	606	TOE	CG'-CH'-OI'-CK'
3	B	604	PG0	OTT-C1-C2-O1
5	A	606	TOE	CD'-CE'-OF'-CG'

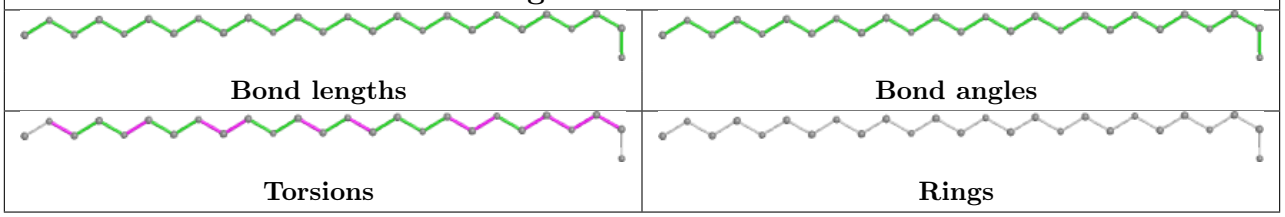
There are no ring outliers.

1 monomer is involved in 1 short contact:

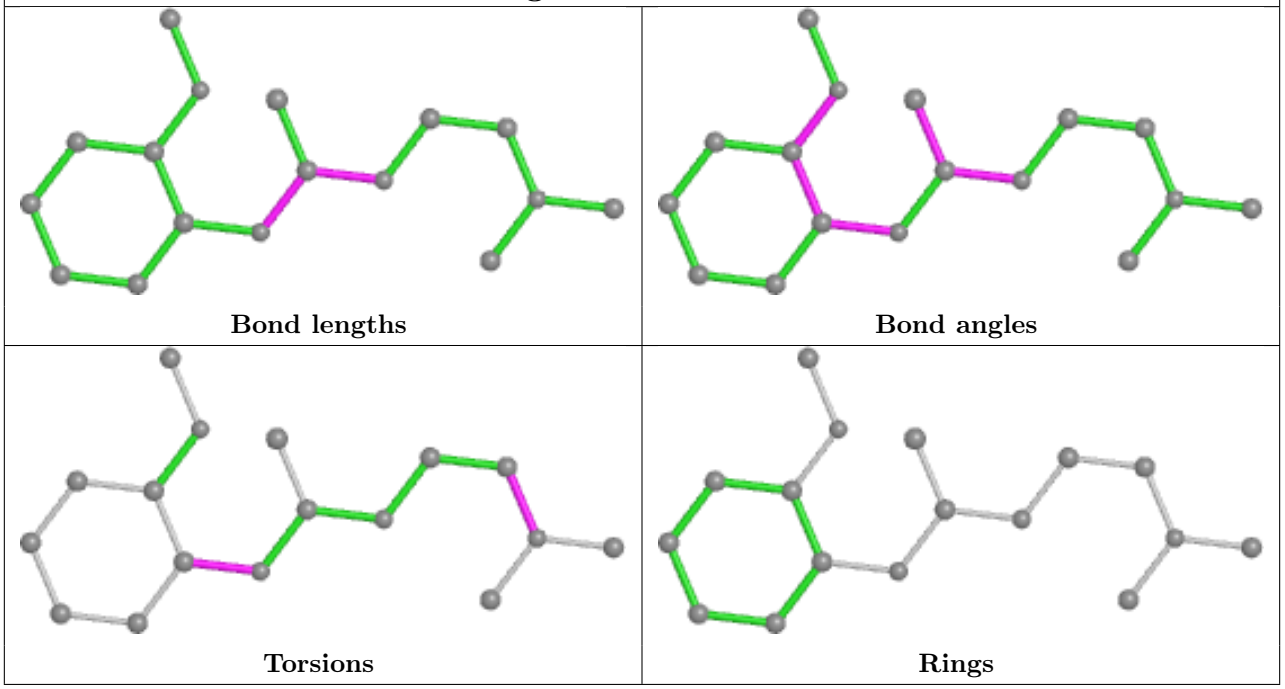
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	7PG	1	0

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.

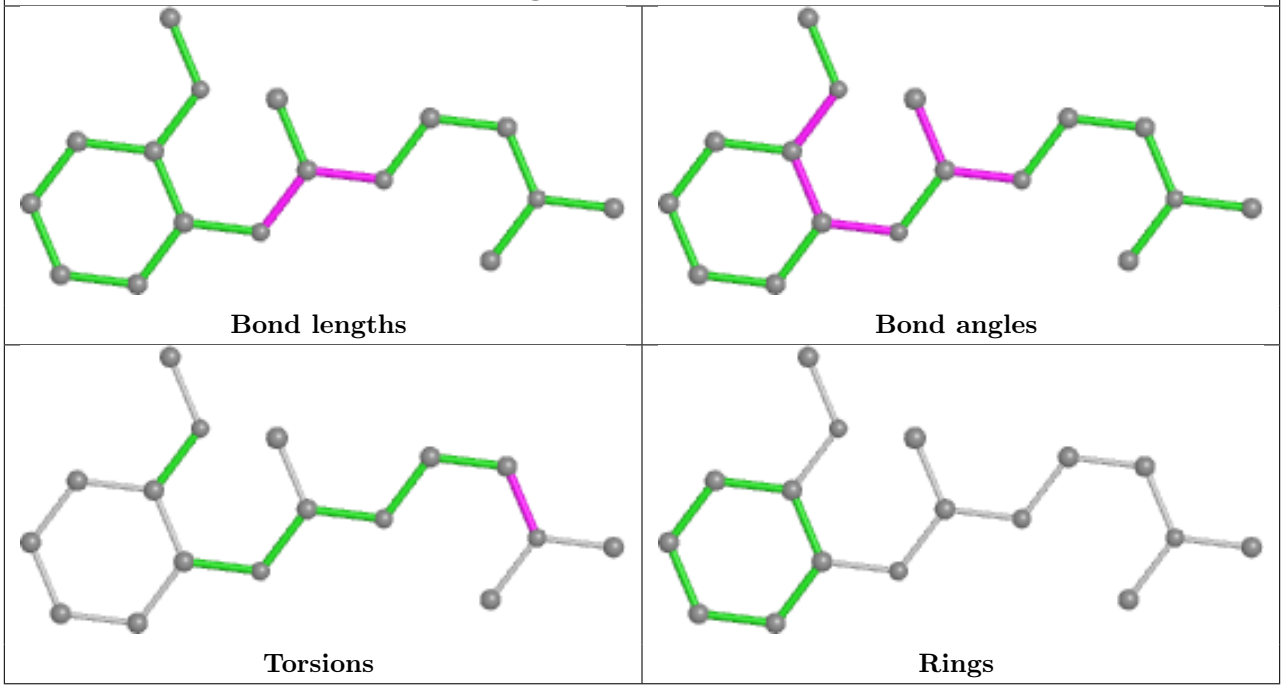
Ligand 7PG B 601



Ligand VY8 A 601



Ligand VY8 B 602



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	536/543 (98%)	-0.10	10 (1%)	66	71	31, 45, 70, 129	0
1	B	534/543 (98%)	0.05	16 (2%)	50	56	34, 50, 75, 129	1 (0%)
All	All	1070/1086 (98%)	-0.03	26 (2%)	59	64	31, 48, 74, 129	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	543	THR	5.8
1	A	495	SER	5.8
1	B	496	LYS	4.9
1	A	540	LEU	4.5
1	A	496	LYS	4.3
1	B	542	ALA	4.1
1	B	4	GLU	3.4
1	B	540	LEU	3.4
1	A	6	PRO	3.2
1	B	105	TYR	3.2
1	B	541	SER	3.1
1	A	493	ARG	3.0
1	A	492	PRO	3.0
1	B	109	ALA	2.9
1	A	541	SER	2.7
1	A	497	SER	2.5
1	A	494	ASP	2.4
1	B	497	SER	2.3
1	B	257	CYS	2.3
1	B	350	ASN	2.3
1	B	495	SER	2.2
1	B	351	GLU	2.1
1	B	9	LEU	2.1
1	B	13	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	268	GLU	2.0
1	B	461	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

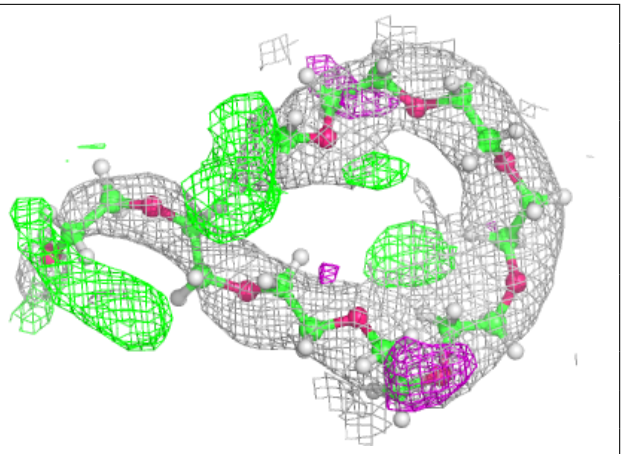
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

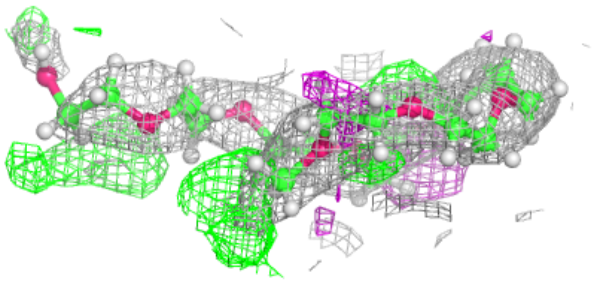
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MXE	B	607	5/5	0.46	0.28	68,82,91,91	0
5	TOE	A	606	11/11	0.49	0.25	64,90,109,113	0
3	PG0	B	604	8/8	0.72	0.40	71,86,102,102	0
3	PG0	A	602	8/8	0.73	0.33	72,87,98,112	0
5	TOE	A	605	11/11	0.78	0.23	60,80,100,107	0
3	PG0	B	605	8/8	0.84	0.16	68,82,95,95	0
4	MXE	A	603	5/5	0.84	0.16	65,79,93,96	0
4	MXE	B	606	5/5	0.84	0.14	60,73,87,87	0
6	7PG	B	601	26/26	0.88	0.20	47,75,100,115	0
3	PG0	B	603	8/8	0.89	0.18	68,89,98,108	0
4	MXE	A	604	5/5	0.89	0.14	63,76,87,87	0
4	MXE	B	608	5/5	0.89	0.17	72,90,96,96	0
2	VY8	B	602	17/17	0.96	0.15	43,59,81,81	0
2	VY8	A	601	17/17	0.97	0.13	33,48,75,75	0

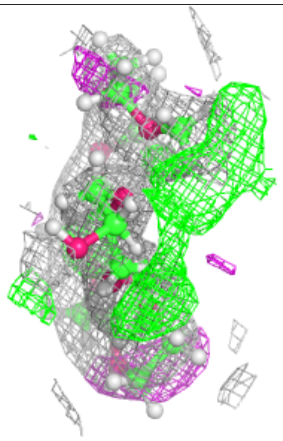
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7PG 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)

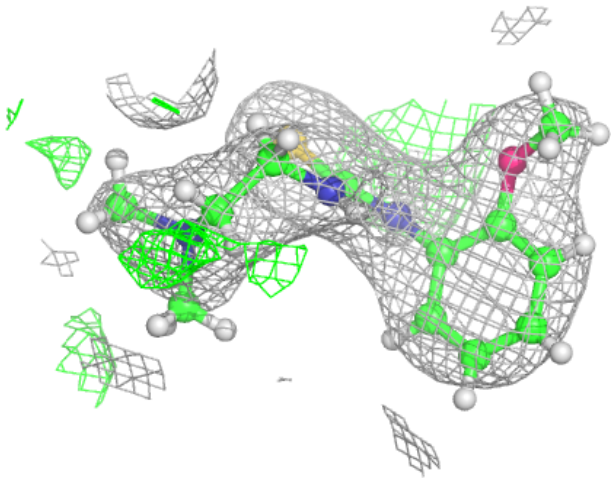


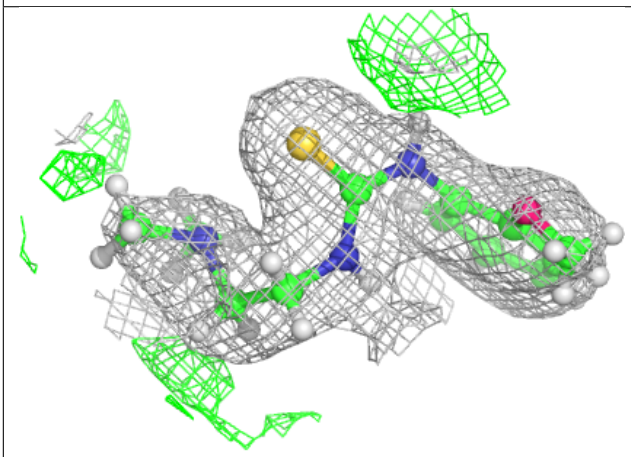


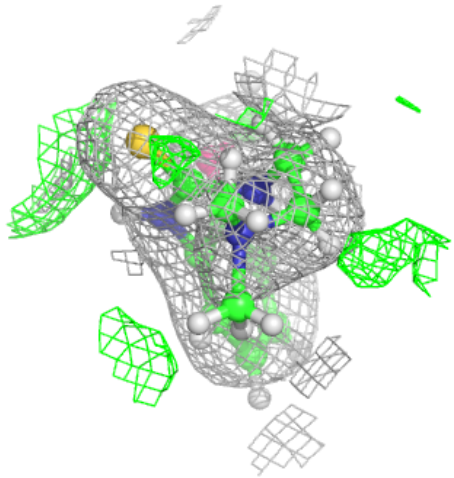


Electron density around VY8 B 602:

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

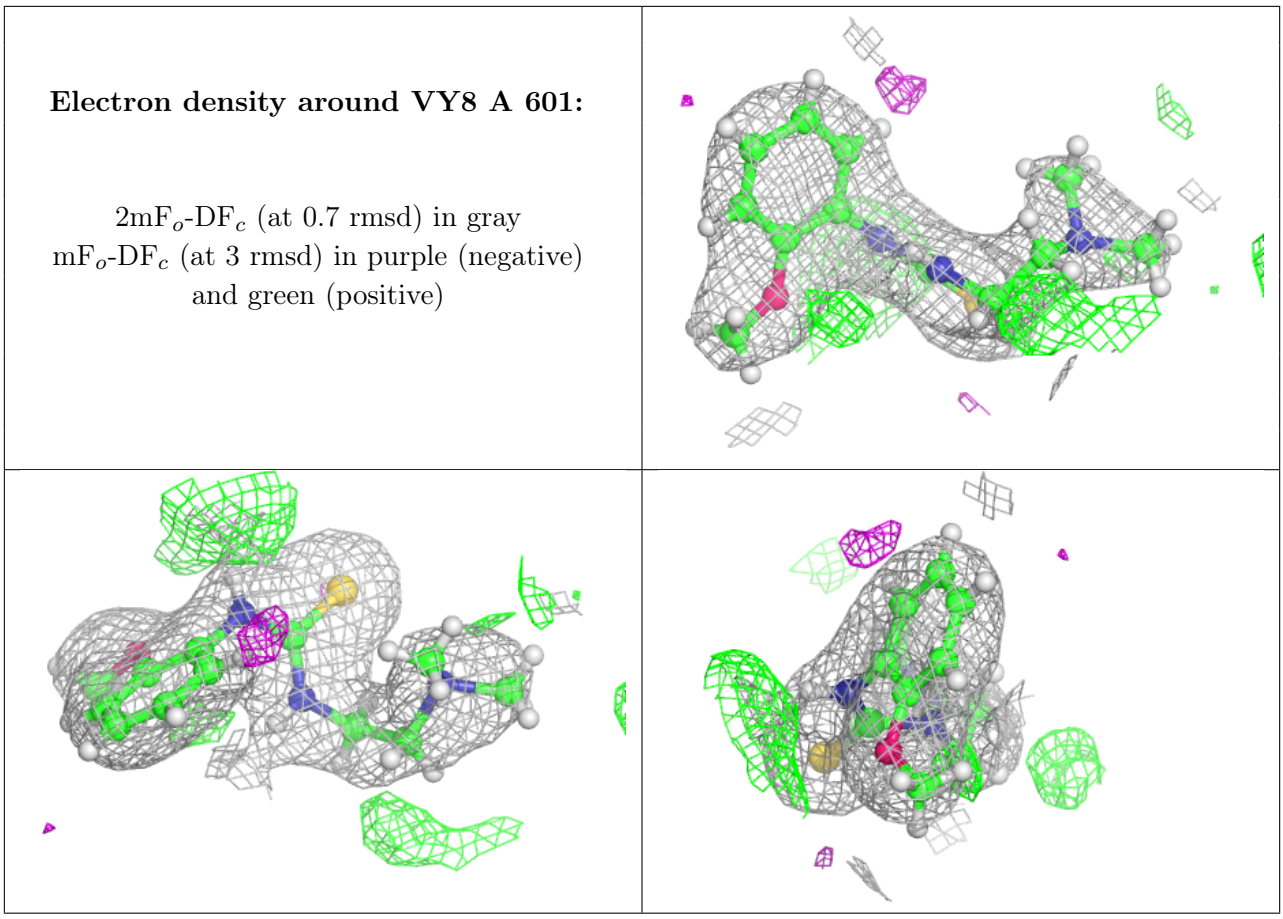






Electron density around VY8 A 601:

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



6.5 Other polymers

There are no such residues in this entry.