Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 01:22 am GMT

PDB ID	:	6RV4
Title	:	Crystal structure of the human two pore domain potassium ion channel TASK-1 (K2P3.1) in a closed conformation with a bound inhibitor BAY 2341237
Authors	:	Rodstrom, K.E.J.; Pike, A.C.W.; Zhang, W.; Quigley, A.; Speedman, D.; Mukhopadhyay, S.M.M.; Shrestha, L.; Chalk, R.; Venkaya, S.; Bushell, S.R.; Tessitore, A.; Burgess-Brown, N.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Carpenter, E.P.; Structural Genomics Consortium (SGC)
Deposited on	:	2019-05-30
Resolution	:	3.10 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

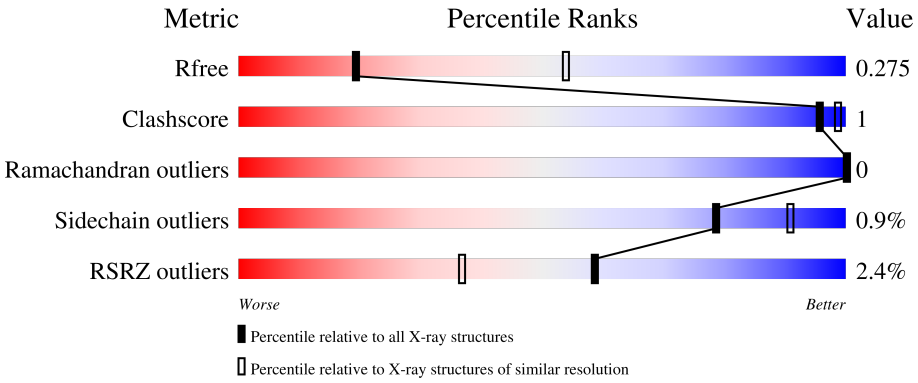
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	264	4% 93%
1	B	264	% 93% 5%
1	C	264	4% 95%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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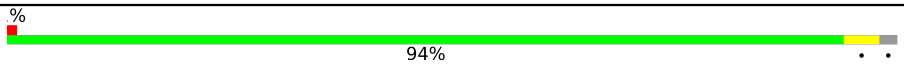
Mol	Chain	Length	Quality of chain
1	D	264	

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
3	Y01	A	306	-	-	-	X
3	Y01	B	302	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8390 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 Potassium channel subfamily K member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1985	1305	319	349	12			
1	B	258	Total	C	N	O	S	0	0	0
			2005	1311	326	356	12			
1	C	257	Total	C	N	O	S	0	0	0
			1981	1307	316	345	13			
1	D	259	Total	C	N	O	S	0	0	0
			2014	1316	327	359	12			

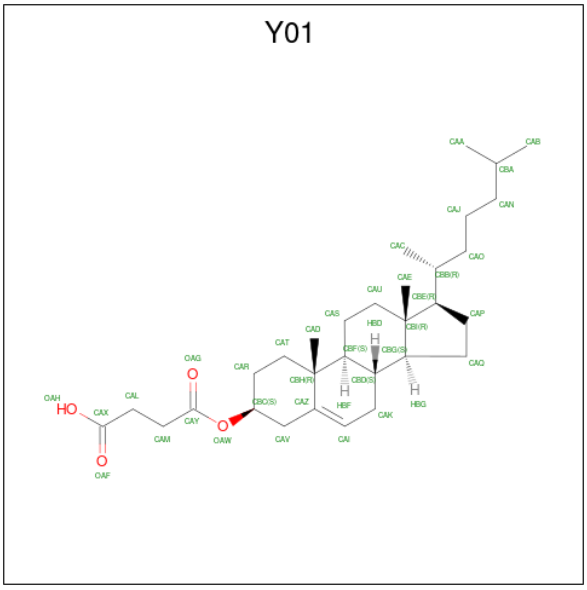
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	ASN	-	expression tag	UNP O14649
A	261	LEU	-	expression tag	UNP O14649
A	262	TYR	-	expression tag	UNP O14649
A	263	PHE	-	expression tag	UNP O14649
A	264	GLN	-	expression tag	UNP O14649
B	260	ASN	-	expression tag	UNP O14649
B	261	LEU	-	expression tag	UNP O14649
B	262	TYR	-	expression tag	UNP O14649
B	263	PHE	-	expression tag	UNP O14649
B	264	GLN	-	expression tag	UNP O14649
C	260	ASN	-	expression tag	UNP O14649
C	261	LEU	-	expression tag	UNP O14649
C	262	TYR	-	expression tag	UNP O14649
C	263	PHE	-	expression tag	UNP O14649
C	264	GLN	-	expression tag	UNP O14649
D	260	ASN	-	expression tag	UNP O14649
D	261	LEU	-	expression tag	UNP O14649
D	262	TYR	-	expression tag	UNP O14649
D	263	PHE	-	expression tag	UNP O14649
D	264	GLN	-	expression tag	UNP O14649

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

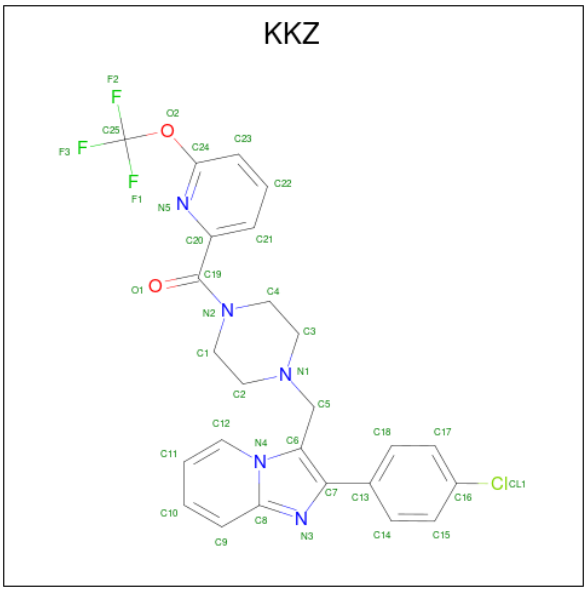
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total K 4 4	0	0
2	C	4	Total K 4 4	0	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



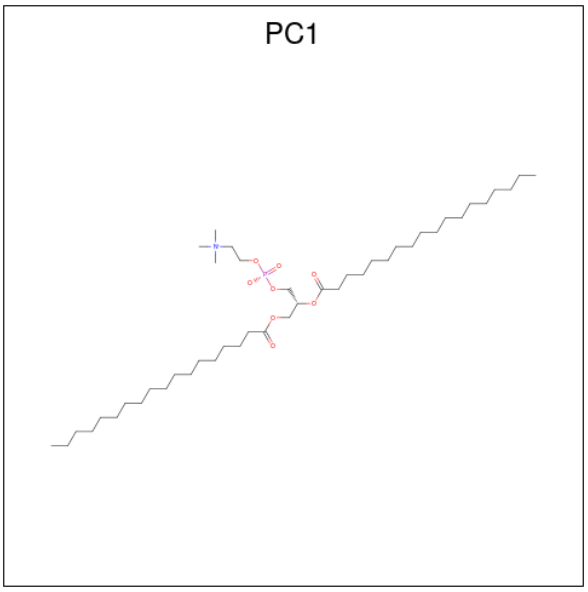
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 35 31 4	0	0
3	A	1	Total C O 35 31 4	0	0
3	A	1	Total C O 35 31 4	0	0
3	B	1	Total C O 35 31 4	0	0
3	C	1	Total C O 35 31 4	0	0
3	D	1	Total C O 35 31 4	0	0

- Molecule 4 is [4-[[2-(4-chlorophenyl)imidazo[1,2-a]pyridin-3-yl]methyl]piperazin-1-yl]-[6-(trifluoromethyloxy)pyridin-2-yl]methanone (three-letter code: KKZ) (formula: $C_{25}H_{21}ClF_3N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			36	25	1	3	5	2		
4	D	1	Total	C	Cl	F	N	O	0	0
			36	25	1	3	5	2		

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			38	34	4		

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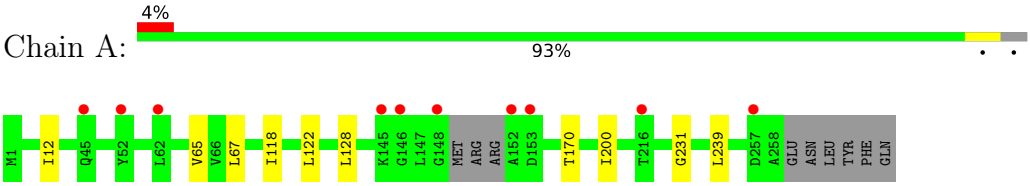
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 18 16 2	0	0
5	C	1	Total C O 21 19 2	0	0
5	C	1	Total C O 38 34 4	0	0

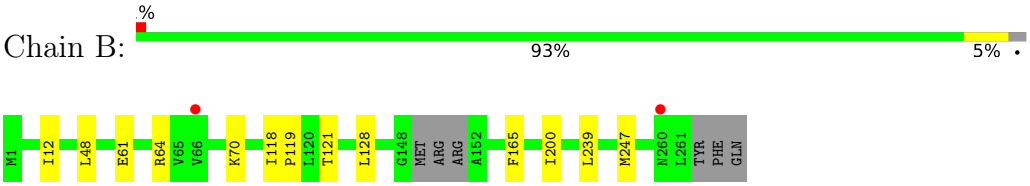
3 Residue-property plots (i)

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.

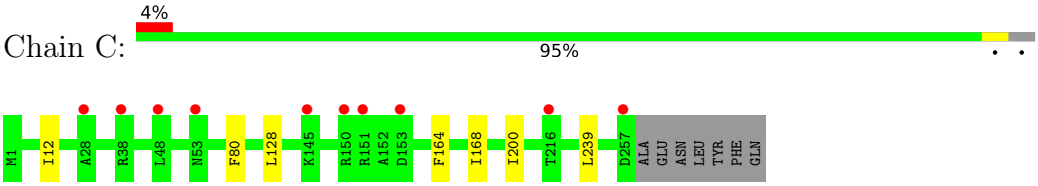
• Molecule 1: Potassium channel subfamily K member 3



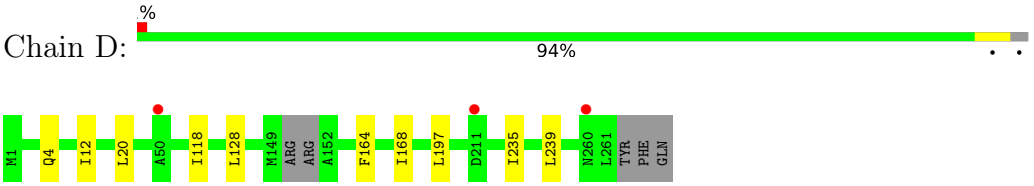
• Molecule 1: Potassium channel subfamily K member 3



• Molecule 1: Potassium channel subfamily K member 3



• Molecule 1: Potassium channel subfamily K member 3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.10Å 201.33Å 238.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.16 – 3.10 43.12 – 3.10	Depositor EDS
% Data completeness (in resolution range)	80.9 (41.16-3.10) 80.9 (43.12-3.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.250 , 0.256 0.269 , 0.275	Depositor DCC
R_{free} test set	1587 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.2	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	0.81	EDS
Total number of atoms	8390	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.74% 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: PC1, K, Y01, KKZ

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	0.41	0/2030	0.57	0/2755
1	B	0.42	0/2050	0.56	0/2783
1	C	0.41	0/2027	0.56	0/2751
1	D	0.41	0/2059	0.56	0/2795
All	All	0.41	0/8166	0.56	0/11084

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1985	0	1954	8	0
1	B	2005	0	1962	9	0
1	C	1981	0	1940	5	0
1	D	2014	0	1968	6	0
2	A	4	0	0	0	0
2	C	4	0	0	0	0
3	A	105	0	147	1	0
3	B	35	0	49	0	0
3	C	35	0	49	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	35	0	49	0	0
4	A	36	0	0	0	0
4	D	36	0	0	0	0
5	A	38	0	60	0	0
5	B	18	0	26	0	0
5	C	59	0	95	0	0
All	All	8390	0	8299	18	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 1.

All (18) 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:C:80:PHE:HZ	1:D:20:LEU:HD23	1.70	0.57
1:A:12:ILE:HD11	1:B:128:LEU:HD13	1.95	0.48
1:A:200:ILE:HD11	1:B:118:ILE:HD11	1.95	0.47
1:A:67:LEU:HD22	1:B:70:LYS:HD3	1.96	0.47
1:A:65:VAL:HG21	1:B:48:LEU:HD12	1.97	0.46
1:C:12:ILE:HD11	1:D:128:LEU:HD13	1.97	0.45
1:A:118:ILE:HD11	1:B:200:ILE:HD11	1.97	0.45
1:D:197:LEU:HB3	1:D:235:ILE:HG13	1.97	0.45
1:C:200:ILE:HD11	1:D:118:ILE:HD11	2.00	0.43
1:A:170:THR:HG21	1:A:231:GLY:HA2	2.02	0.42
1:A:128:LEU:HD13	1:B:12:ILE:HD11	2.02	0.42
3:A:305:Y01:HAJ2	1:B:119:PRO:HG2	2.02	0.42
1:A:122:LEU:HB3	1:B:247:MET:HE2	2.01	0.41
1:B:61:GLU:HG2	1:B:64:ARG:NH2	2.35	0.41
1:D:164:PHE:CE2	1:D:168:ILE:HD11	2.56	0.41
1:C:164:PHE:CE2	1:C:168:ILE:HD11	2.56	0.41
3:C:308:Y01:HAU2	3:C:308:Y01:HAC1	2.03	0.41
1:C:128:LEU:HD13	1:D:12:ILE:HD11	2.03	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	251/264 (95%)	245 (98%)	6 (2%)	0	100	100
1	B	254/264 (96%)	248 (98%)	6 (2%)	0	100	100
1	C	255/264 (97%)	248 (97%)	7 (3%)	0	100	100
1	D	255/264 (97%)	249 (98%)	6 (2%)	0	100	100
All	All	1015/1056 (96%)	990 (98%)	25 (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	198/221 (90%)	197 (100%)	1 (0%)	88	94
1	B	201/221 (91%)	198 (98%)	3 (2%)	65	85
1	C	193/221 (87%)	192 (100%)	1 (0%)	88	94
1	D	202/221 (91%)	200 (99%)	2 (1%)	76	90
All	All	794/884 (90%)	787 (99%)	7 (1%)	78	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	LEU
1	B	121	THR

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Mol	Chain	Res	Type
1	B	165	PHE
1	B	239	LEU
1	C	239	LEU
1	D	4	GLN
1	D	239	LEU

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

Mol	Chain	Res	Type
1	D	183	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
5	PC1	A	308	-	37,37,53	0.23	0	39,39,61	0.31	0
3	Y01	B	302	-	38,38,38	0.34	0	57,57,57	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	KKZ	A	307	-	37,40,40	1.24	6 (16%)	45,58,58	1.14	3 (6%)
3	Y01	D	303	-	38,38,38	0.36	0	57,57,57	0.42	0
3	Y01	A	306	-	38,38,38	0.34	0	57,57,57	0.45	0
5	PC1	B	303	-	17,17,53	0.24	0	17,17,61	0.24	0
3	Y01	A	305	-	38,38,38	0.34	0	57,57,57	0.40	0
4	KKZ	D	302	-	37,40,40	1.24	6 (16%)	45,58,58	1.16	4 (8%)
5	PC1	C	305	-	20,20,53	0.25	0	20,20,61	0.25	0
3	Y01	C	308	-	38,38,38	0.34	0	57,57,57	0.41	0
3	Y01	A	301	-	38,38,38	0.36	0	57,57,57	0.41	0
5	PC1	C	306	-	37,37,53	0.25	0	39,39,61	0.33	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
5	PC1	A	308	-	-	5/38/38/57	-
3	Y01	B	302	-	-	5/19/77/77	0/4/4/4
4	KKZ	A	307	-	-	5/18/31/31	0/5/5/5
3	Y01	D	303	-	-	5/19/77/77	0/4/4/4
3	Y01	A	306	-	-	5/19/77/77	0/4/4/4
5	PC1	B	303	-	-	3/16/16/57	-
3	Y01	A	305	-	-	5/19/77/77	0/4/4/4
4	KKZ	D	302	-	-	5/18/31/31	0/5/5/5
5	PC1	C	305	-	-	2/19/19/57	-
3	Y01	C	308	-	-	5/19/77/77	0/4/4/4
3	Y01	A	301	-	-	5/19/77/77	0/4/4/4
5	PC1	C	306	-	-	5/38/38/57	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	302	KKZ	C7-C6	3.60	1.49	1.40
4	A	307	KKZ	C7-C6	3.59	1.49	1.40
4	A	307	KKZ	C8-N3	2.36	1.35	1.33
4	D	302	KKZ	C12-N4	-2.35	1.35	1.38
4	A	307	KKZ	C12-N4	-2.35	1.35	1.38
4	D	302	KKZ	C16-CL1	2.31	1.79	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	307	KKZ	C16-CL1	2.27	1.79	1.74
4	D	302	KKZ	C24-N5	2.22	1.36	1.33
4	D	302	KKZ	C8-N3	2.22	1.35	1.33
4	A	307	KKZ	O2-C25	2.18	1.44	1.31
4	D	302	KKZ	O2-C25	2.15	1.43	1.31
4	A	307	KKZ	C24-N5	2.12	1.36	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	307	KKZ	C21-C20-N5	-2.88	119.55	122.92
4	D	302	KKZ	C21-C20-N5	-2.65	119.82	122.92
4	D	302	KKZ	O2-C24-C23	2.57	119.66	115.51
4	A	307	KKZ	O2-C24-C23	2.29	119.20	115.51
4	D	302	KKZ	C3-N1-C2	2.21	113.80	108.83
4	A	307	KKZ	C3-N1-C2	2.18	113.73	108.83
4	D	302	KKZ	O1-C19-C20	-2.01	115.11	119.00

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	307	KKZ	C6-C5-N1-C2
4	A	307	KKZ	C6-C5-N1-C3
4	A	307	KKZ	F2-C25-O2-C24
4	D	302	KKZ	C6-C5-N1-C2
4	D	302	KKZ	C6-C5-N1-C3
4	D	302	KKZ	F2-C25-O2-C24
4	A	307	KKZ	F3-C25-O2-C24
4	D	302	KKZ	F3-C25-O2-C24
3	A	306	Y01	CAJ-CAO-CBB-CAC
3	B	302	Y01	CAJ-CAO-CBB-CAC
3	A	306	Y01	CAJ-CAO-CBB-CBE
3	B	302	Y01	CAJ-CAO-CBB-CBE
5	C	306	PC1	C26-C27-C28-C29
4	A	307	KKZ	F1-C25-O2-C24
4	D	302	KKZ	F1-C25-O2-C24
5	B	303	PC1	C21-C22-C23-C24
5	C	306	PC1	C31-C32-C33-C34
5	A	308	PC1	C31-C32-C33-C34
5	C	305	PC1	C21-C22-C23-C24
5	C	305	PC1	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
5	C	306	PC1	C39-C3A-C3B-C3C
5	A	308	PC1	C39-C3A-C3B-C3C
5	B	303	PC1	C28-C29-C2A-C2B
5	A	308	PC1	C21-C22-C23-C24
5	C	306	PC1	C24-C25-C26-C27
3	D	303	Y01	CAJ-CAO-CBB-CBE
5	A	308	PC1	C24-C25-C26-C27
5	B	303	PC1	C29-C2A-C2B-C2C
3	A	301	Y01	CAJ-CAO-CBB-CBE
5	A	308	PC1	C2A-C2B-C2C-C2D
3	A	305	Y01	CAJ-CAO-CBB-CBE
3	C	308	Y01	CAJ-CAO-CBB-CBE
5	C	306	PC1	C2A-C2B-C2C-C2D
3	C	308	Y01	CAM-CAL-CAX-OAF
3	C	308	Y01	CAM-CAL-CAX-OAH
3	B	302	Y01	CAM-CAL-CAX-OAH
3	A	306	Y01	CAN-CAJ-CAO-CBB
3	B	302	Y01	CAN-CAJ-CAO-CBB
3	A	306	Y01	CAM-CAL-CAX-OAH
3	D	303	Y01	CAM-CAL-CAX-OAH
3	A	306	Y01	CAM-CAL-CAX-OAF
3	B	302	Y01	CAM-CAL-CAX-OAF
3	D	303	Y01	CAM-CAL-CAX-OAF
3	A	301	Y01	CAM-CAL-CAX-OAH
3	A	305	Y01	CAM-CAL-CAX-OAH
3	A	305	Y01	CAL-CAM-CAY-OAW
3	A	301	Y01	CAM-CAL-CAX-OAF
3	C	308	Y01	CAL-CAM-CAY-OAW
3	A	305	Y01	CAM-CAL-CAX-OAF
3	A	301	Y01	CAL-CAM-CAY-OAW
3	D	303	Y01	CAL-CAM-CAY-OAW
3	D	303	Y01	CAJ-CAO-CBB-CAC
3	A	301	Y01	CAL-CAM-CAY-OAG
3	C	308	Y01	CAL-CAM-CAY-OAG
3	A	305	Y01	CAL-CAM-CAY-OAG

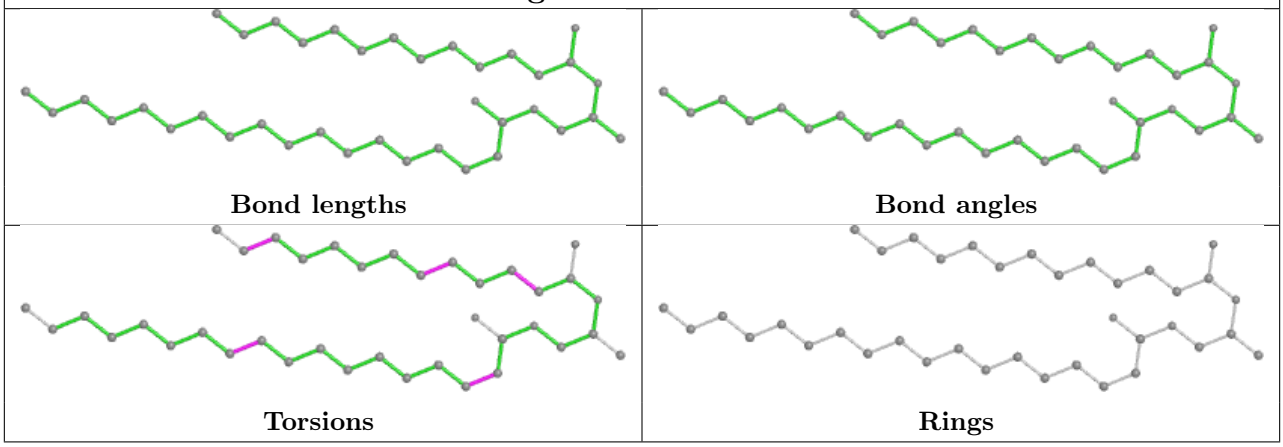
There are no ring outliers.

2 monomers are involved in 2 short contacts:

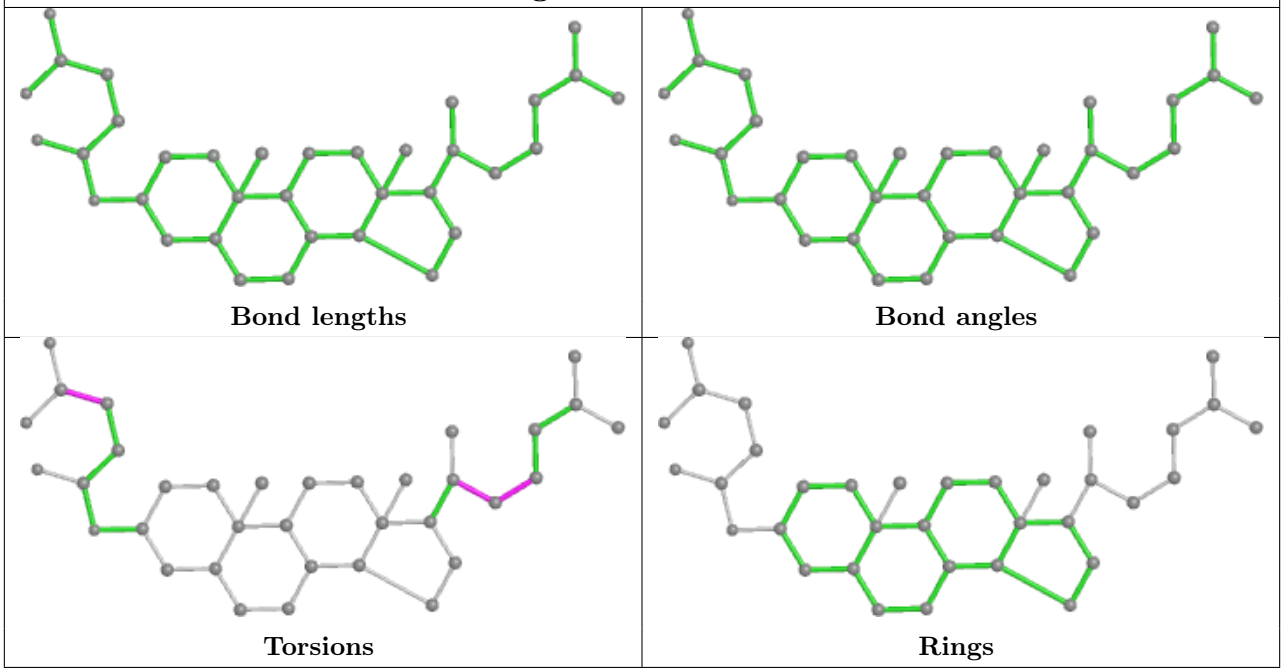
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	305	Y01	1	0
3	C	308	Y01	1	0

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.

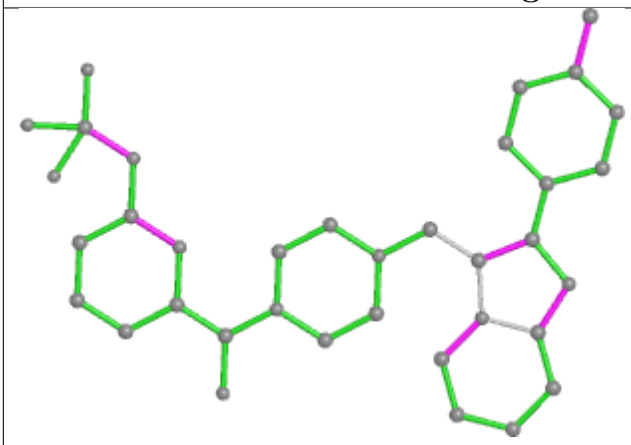
Ligand PC1 A 308



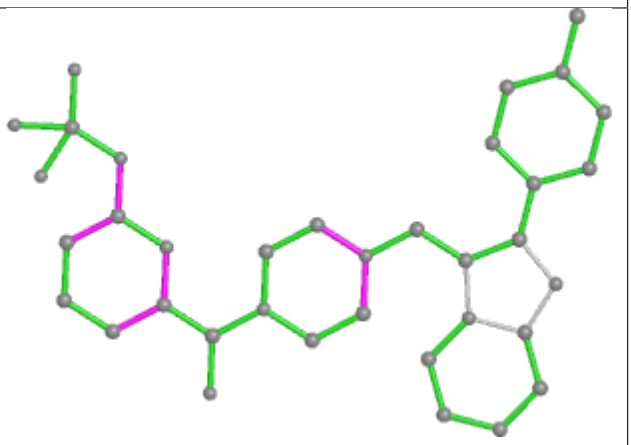
Ligand Y01 B 302



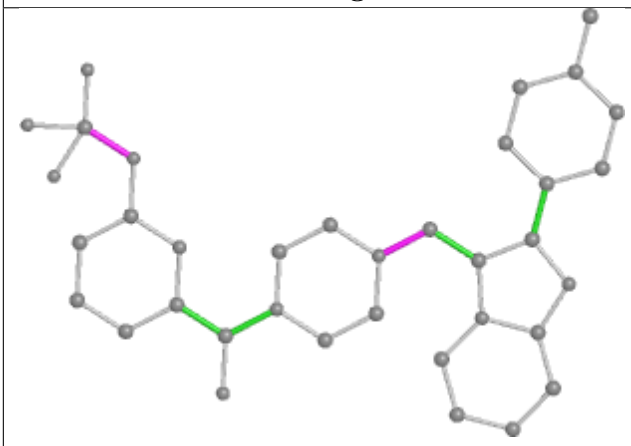
Ligand KKZ A 307



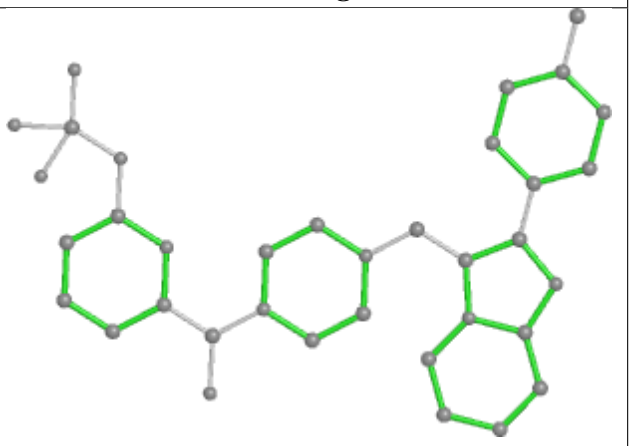
Bond lengths



Bond angles

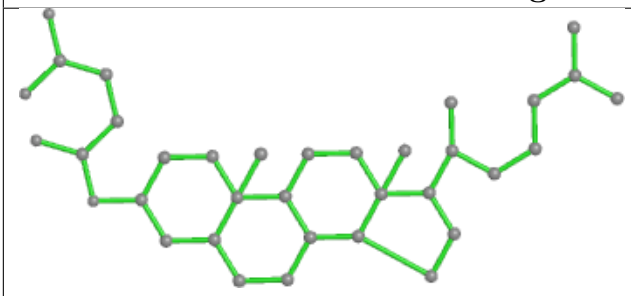


Torsions

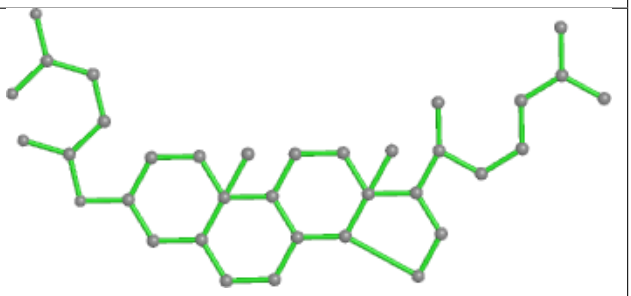


Rings

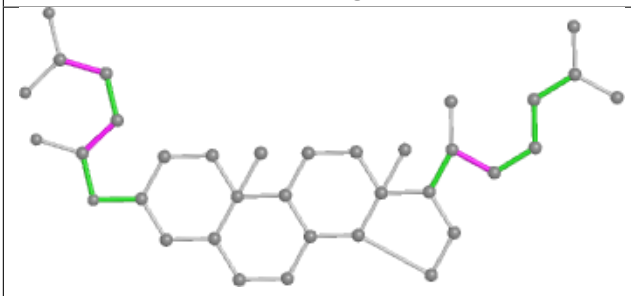
Ligand Y01 D 303



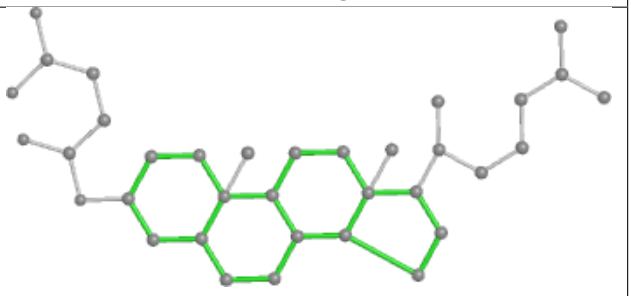
Bond lengths



Bond angles

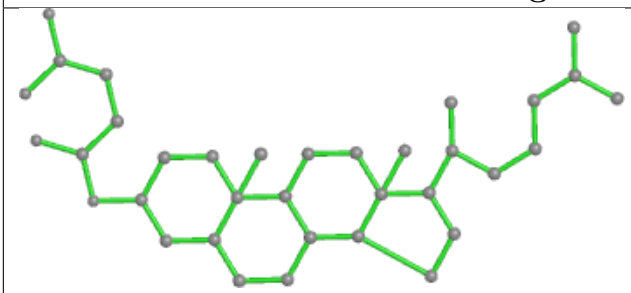


Torsions

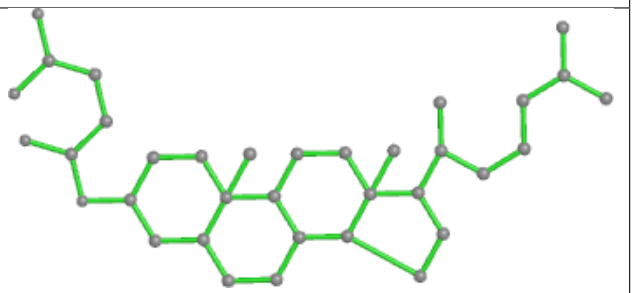


Rings

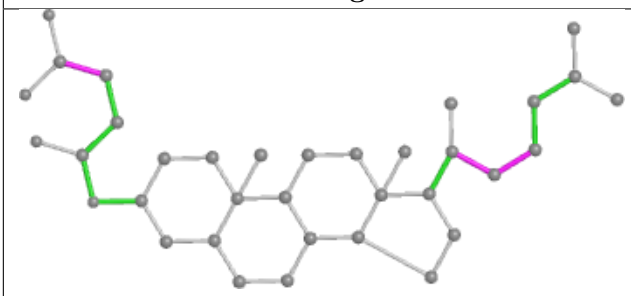
Ligand Y01 A 306



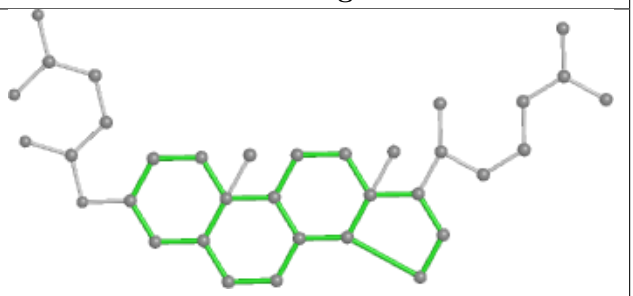
Bond lengths



Bond angles

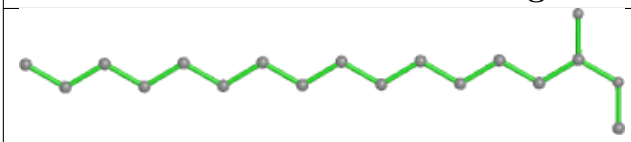


Torsions

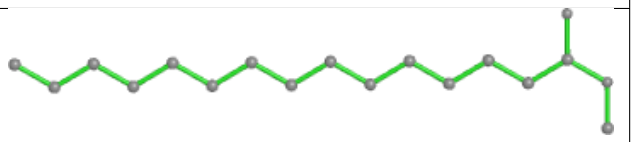


Rings

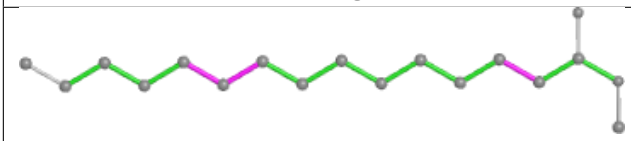
Ligand PC1 B 303



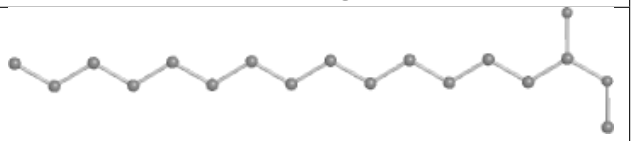
Bond lengths



Bond angles

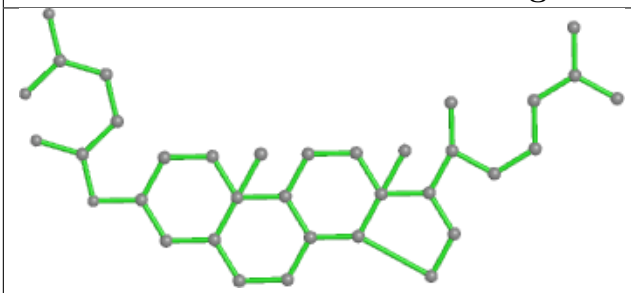


Torsions

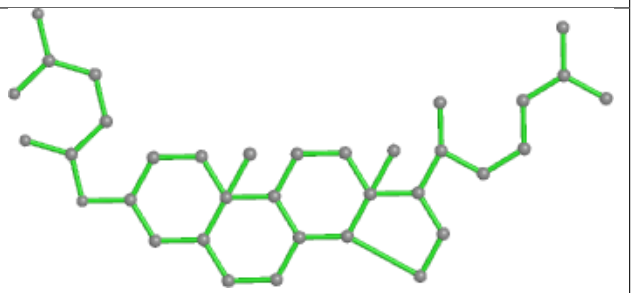


Rings

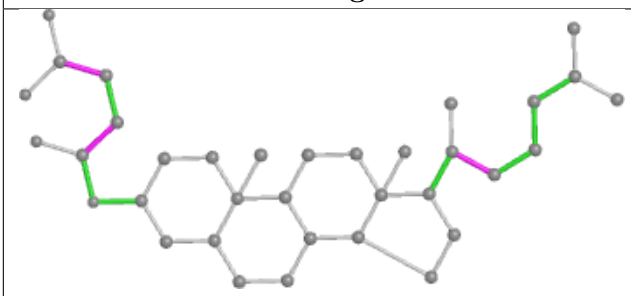
Ligand Y01 A 305



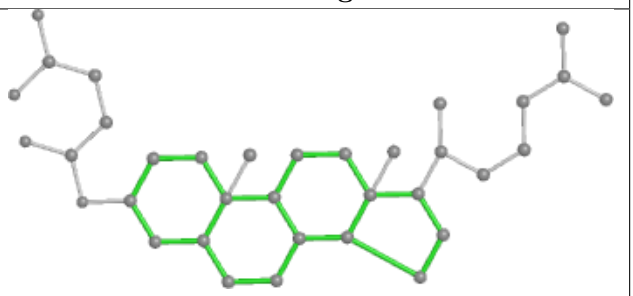
Bond lengths



Bond angles

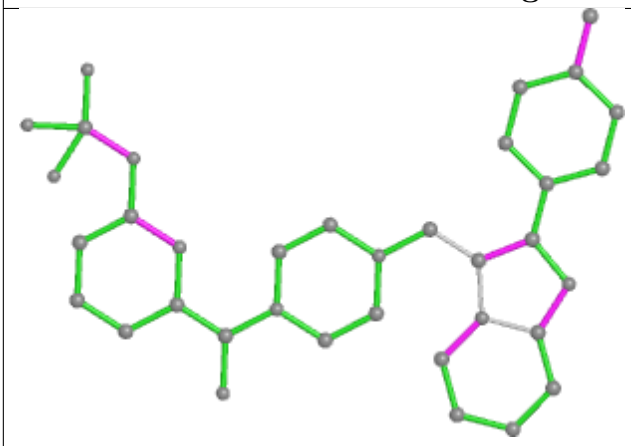


Torsions

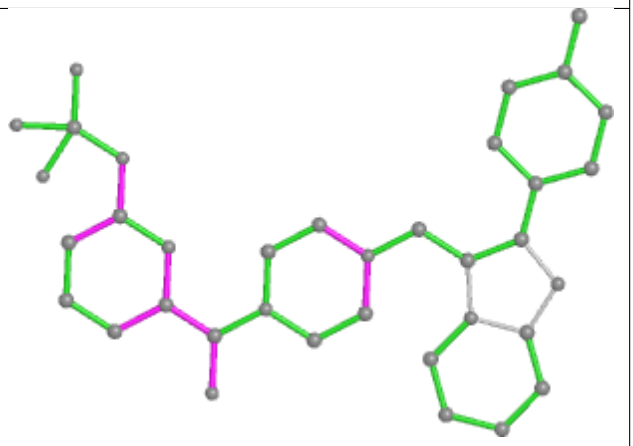


Rings

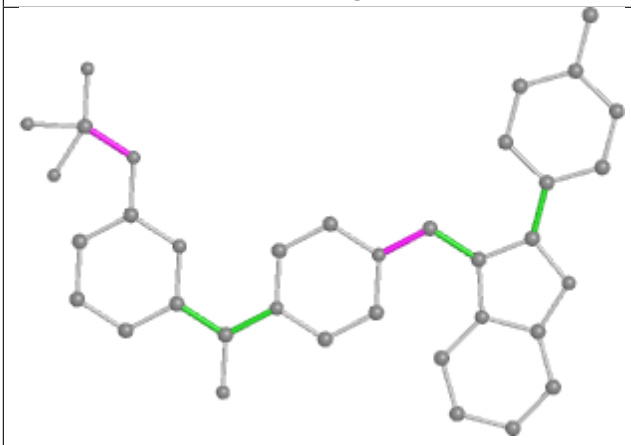
Ligand KKZ D 302



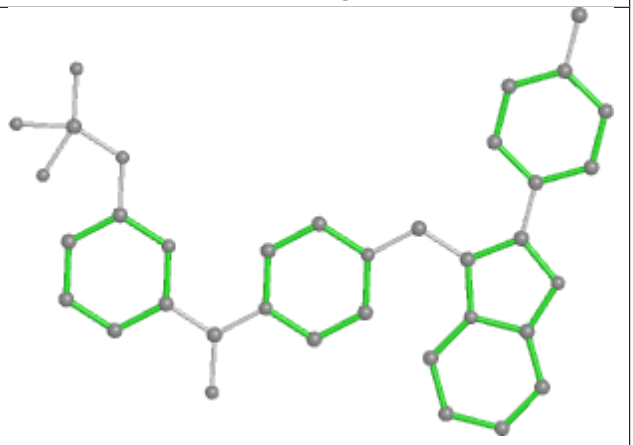
Bond lengths



Bond angles

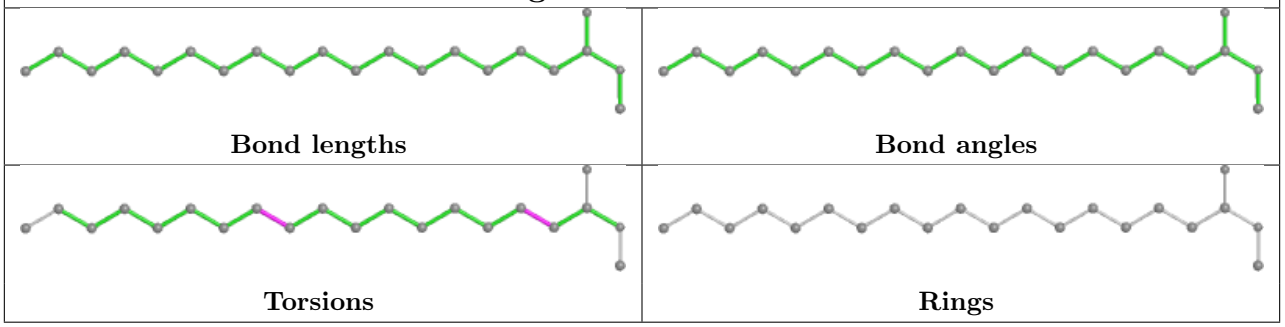


Torsions

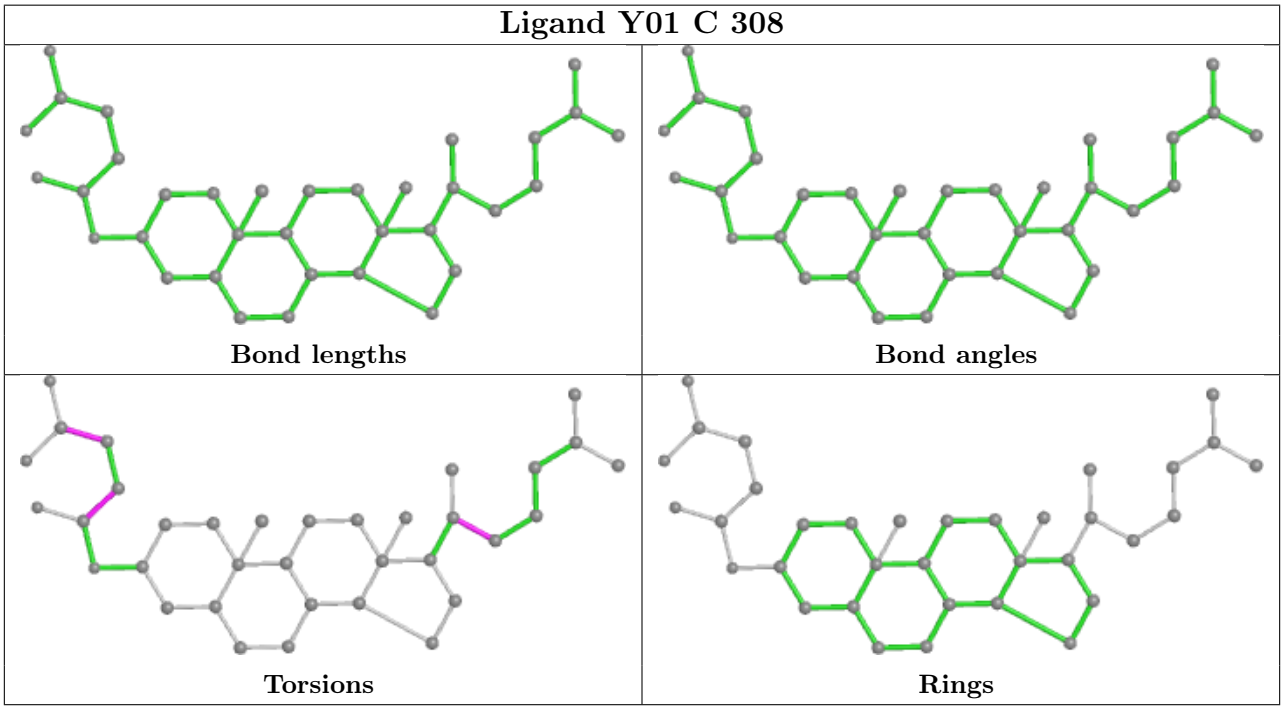


Rings

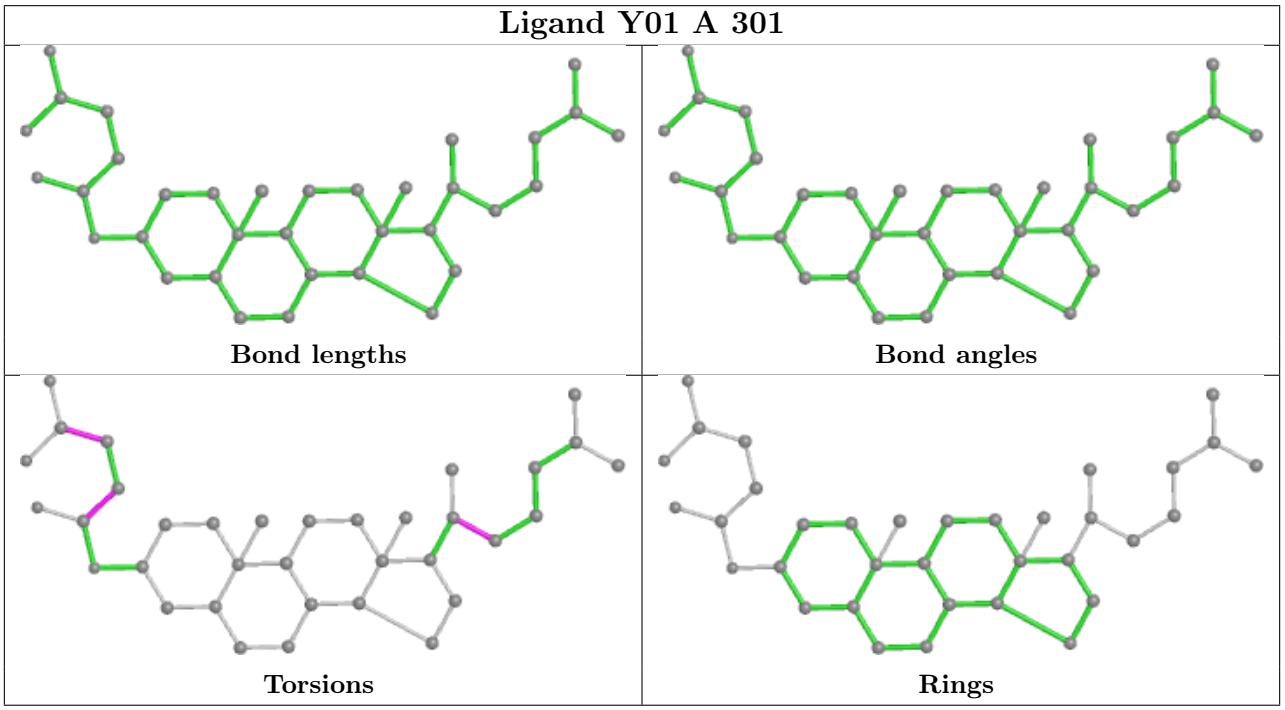
Ligand PC1 C 305

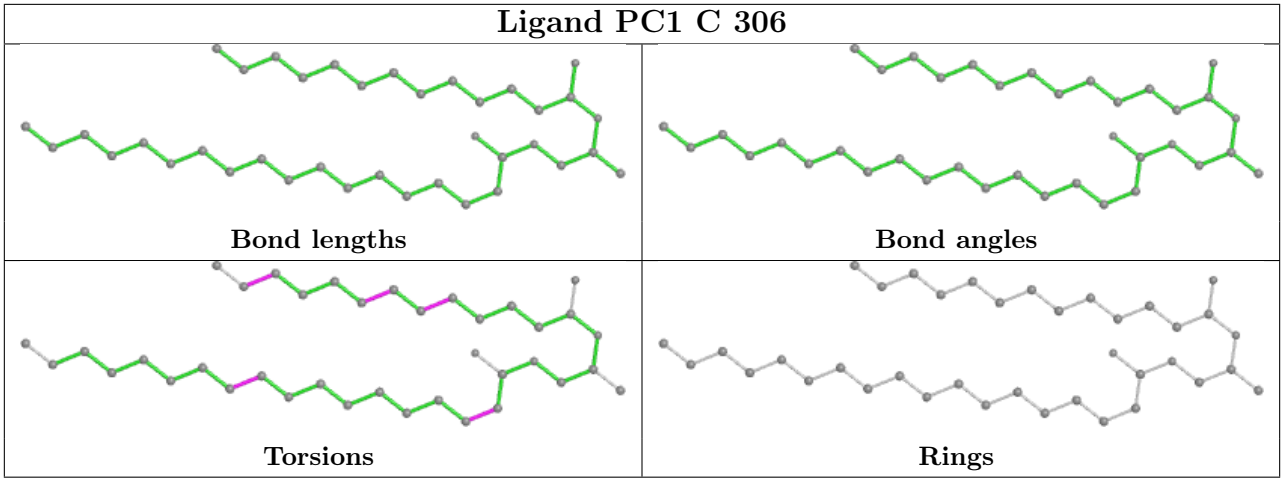


Ligand Y01 C 308



Ligand Y01 A 301





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	255/264 (96%)	0.02	10 (3%) 39 20	13, 40, 93, 125	0
1	B	258/264 (97%)	-0.12	2 (0%) 86 72	15, 42, 85, 125	0
1	C	257/264 (97%)	0.07	10 (3%) 39 20	18, 44, 90, 106	0
1	D	259/264 (98%)	0.01	3 (1%) 79 61	19, 44, 85, 104	0
All	All	1029/1056 (97%)	-0.00	25 (2%) 59 37	13, 43, 87, 125	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	ASN	4.9
1	C	150	ARG	4.8
1	A	153	ASP	4.0
1	D	50	ALA	3.4
1	A	152	ALA	3.2
1	A	216	THR	2.7
1	A	257	ASP	2.6
1	A	145	LYS	2.5
1	B	66	VAL	2.5
1	A	52	TYR	2.4
1	D	260	ASN	2.3
1	C	38	ARG	2.3
1	C	145	LYS	2.3
1	A	148	GLY	2.2
1	C	48	LEU	2.2
1	C	216	THR	2.1
1	C	151	ARG	2.1
1	C	153	ASP	2.1
1	A	146	GLY	2.1
1	C	257	ASP	2.1
1	C	28	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	62	LEU	2.0
1	D	211	ASP	2.0
1	B	260	ASN	2.0
1	A	45	GLN	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
5	PC1	C	306	38/54	0.61	0.35	42,61,76,77	0
5	PC1	A	308	38/54	0.71	0.32	35,57,68,68	0
5	PC1	B	303	18/54	0.72	0.39	75,77,87,87	0
3	Y01	A	306	35/35	0.74	0.44	58,62,70,71	0
3	Y01	B	302	35/35	0.79	0.49	78,79,81,81	0
5	PC1	C	305	21/54	0.83	0.24	34,39,47,47	0
4	KKZ	D	302	36/36	0.85	0.39	74,75,81,81	0
2	K	C	302	1/1	0.87	0.25	105,105,105,105	0
4	KKZ	A	307	36/36	0.90	0.27	38,43,45,45	0
3	Y01	A	305	35/35	0.90	0.28	27,31,46,46	0
3	Y01	C	308	35/35	0.90	0.22	20,33,47,47	0
2	K	A	304	1/1	0.91	0.07	20,20,20,20	0
3	Y01	A	301	35/35	0.91	0.26	37,39,40,40	0
3	Y01	D	303	35/35	0.91	0.27	32,39,52,53	0
2	K	C	304	1/1	0.94	0.13	39,39,39,39	0
2	K	C	303	1/1	0.95	0.09	10,10,10,10	0
2	K	C	307	1/1	0.95	0.06	25,25,25,25	0
2	K	A	303	1/1	0.96	0.15	32,32,32,32	0
2	K	A	302	1/1	0.96	0.25	49,49,49,49	0

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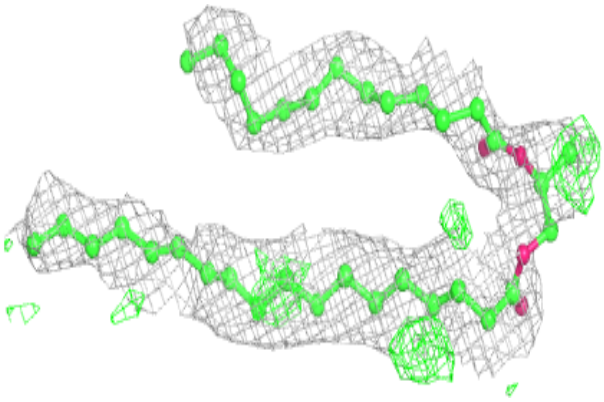
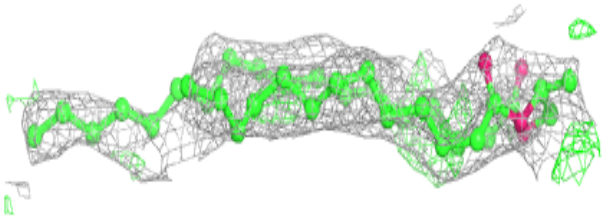
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	K	A	309	1/1	0.98	0.06	19,19,19,19	0

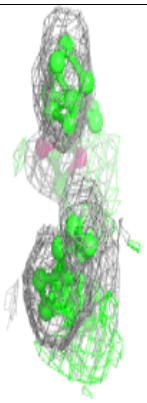
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PC1 C 306:

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

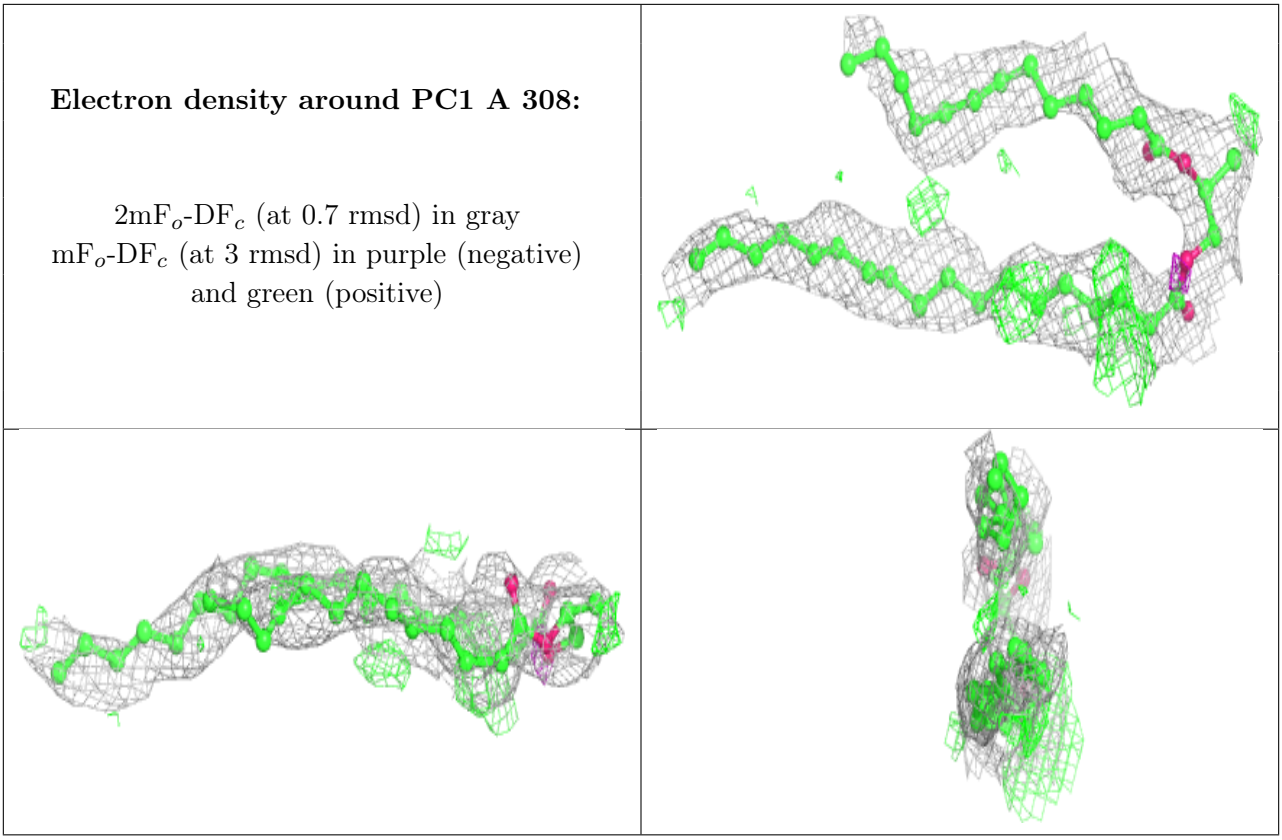






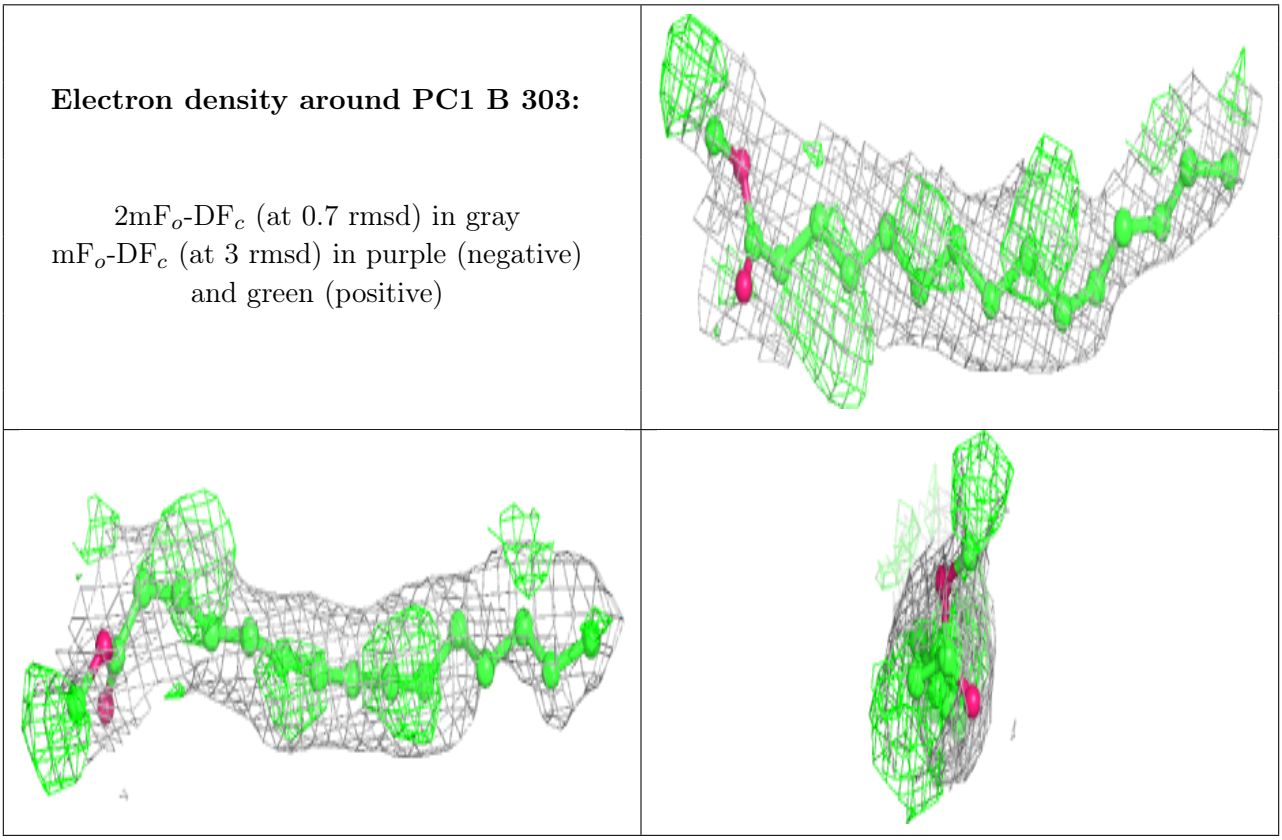
Electron density around PC1 A 308:

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



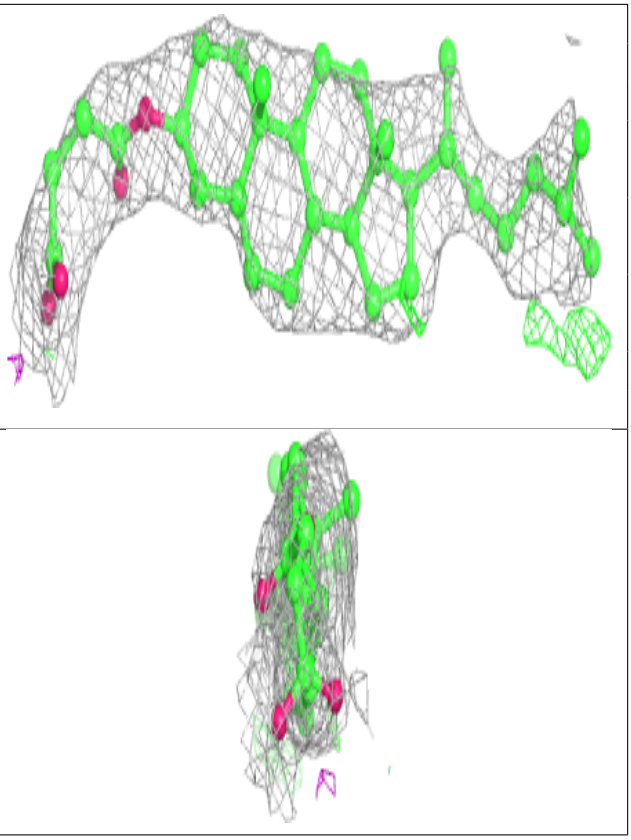
Electron density around PC1 B 303:

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



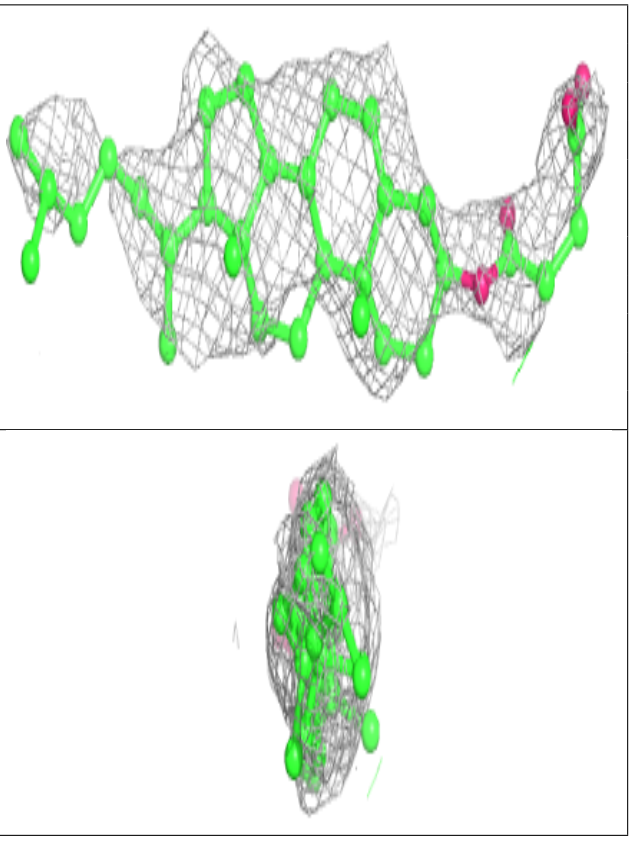
Electron density around Y01 A 306:

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



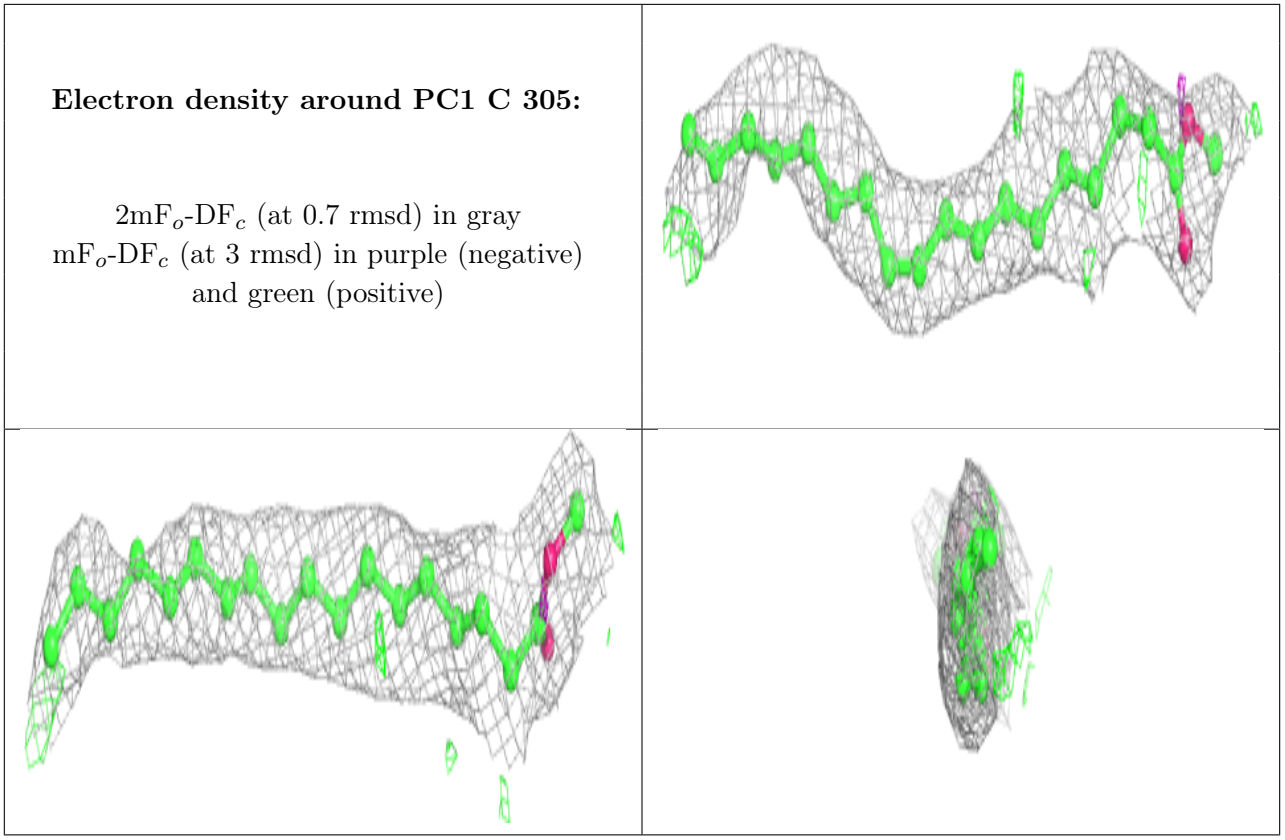
Electron density around Y01 B 302:

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



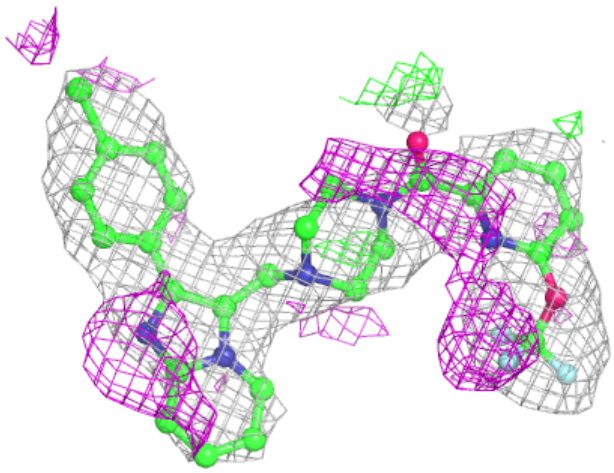
Electron density around PC1 C 305:

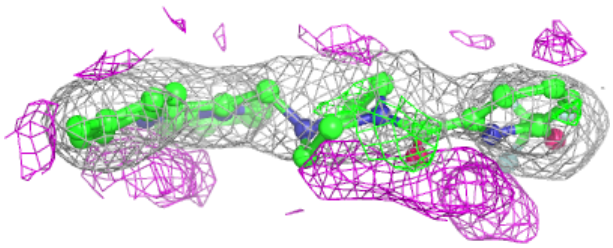
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

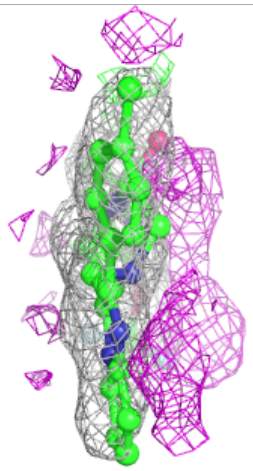


Electron density around KKZ D 302:

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

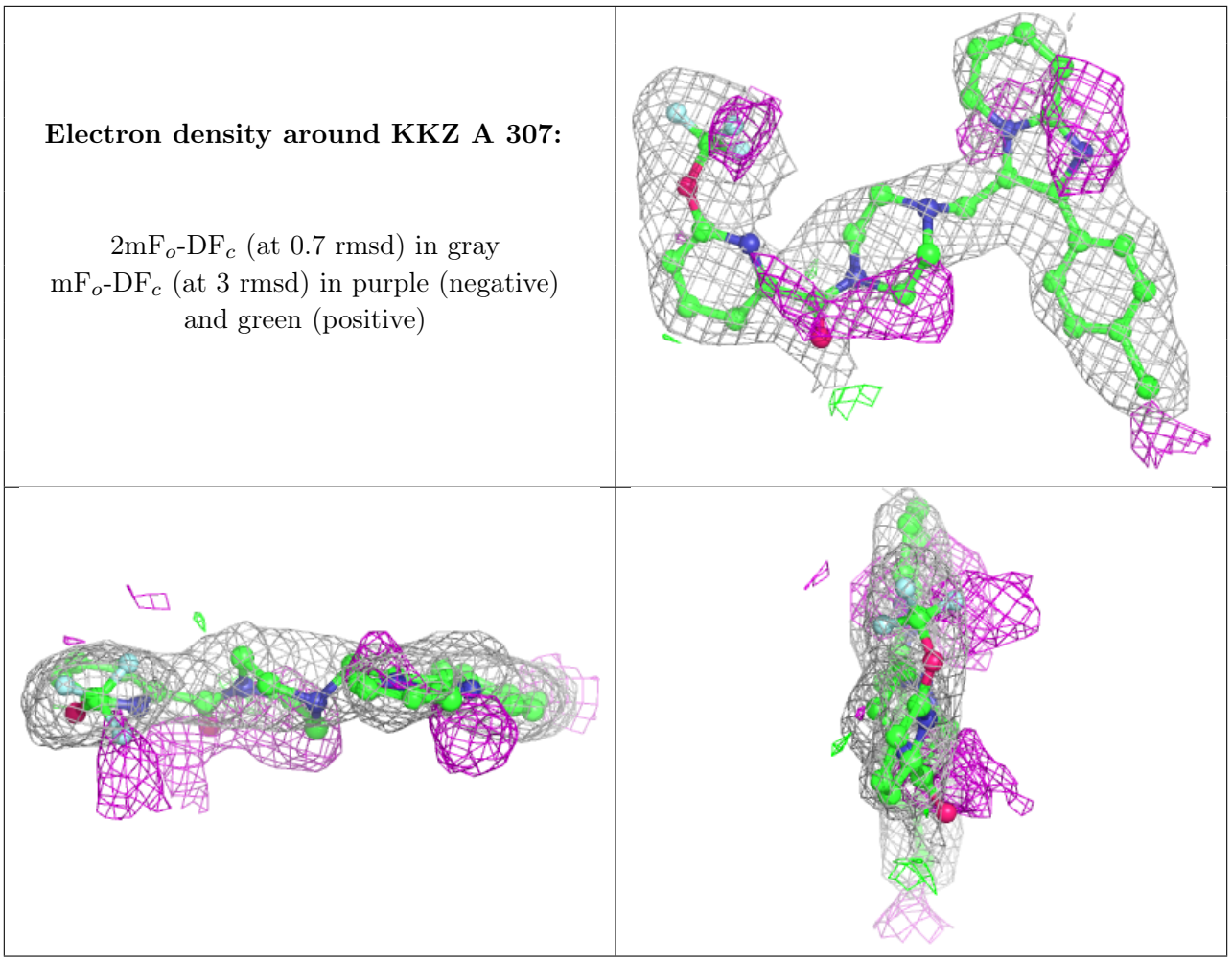






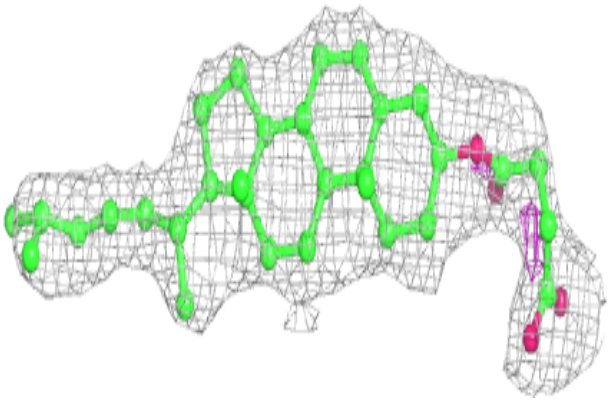
Electron density around KKZ A 307:

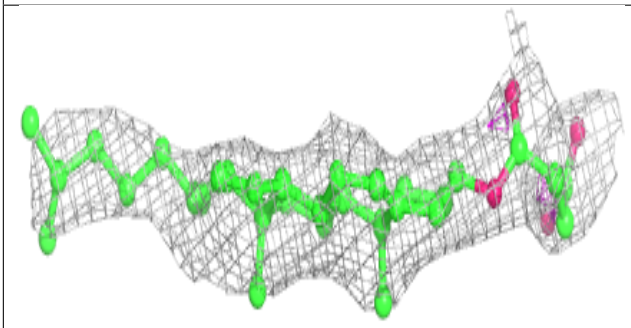
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

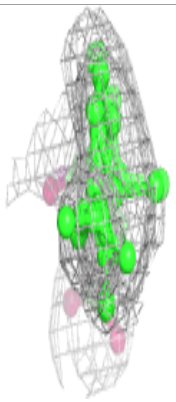


Electron density around Y01 A 305:

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

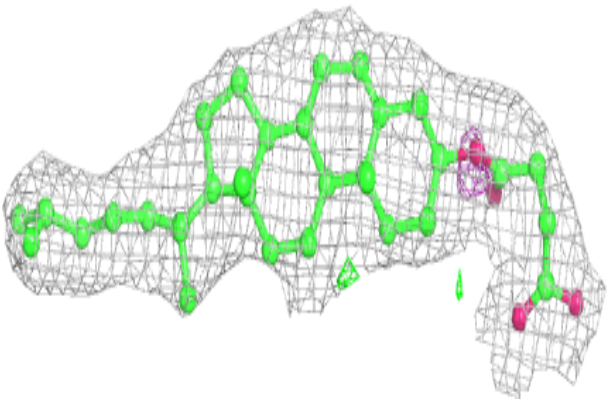


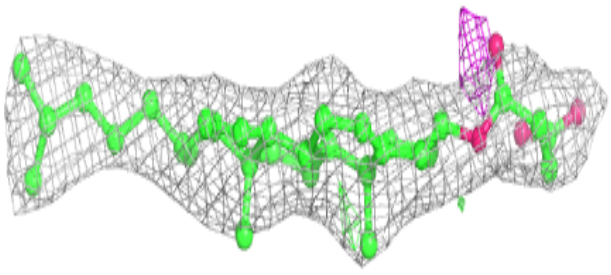


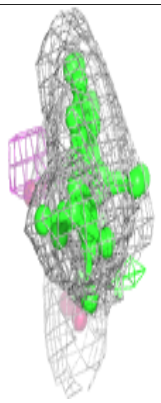


Electron density around Y01 C 308:

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

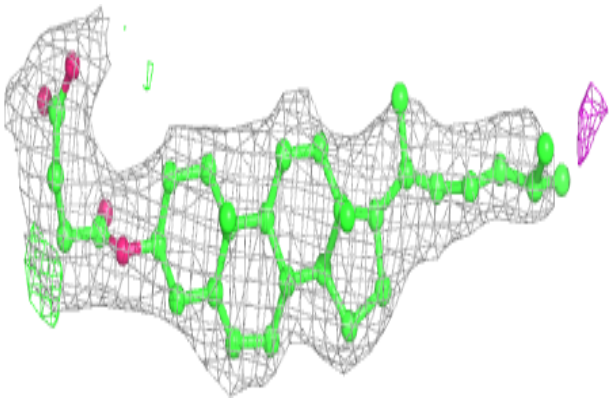


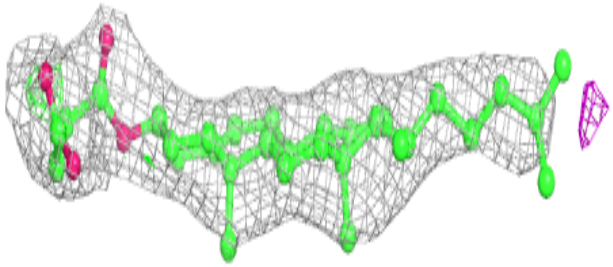


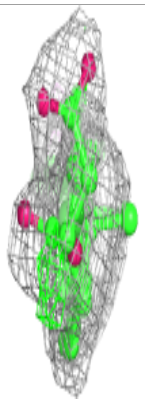


Electron density around Y01 A 301:

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

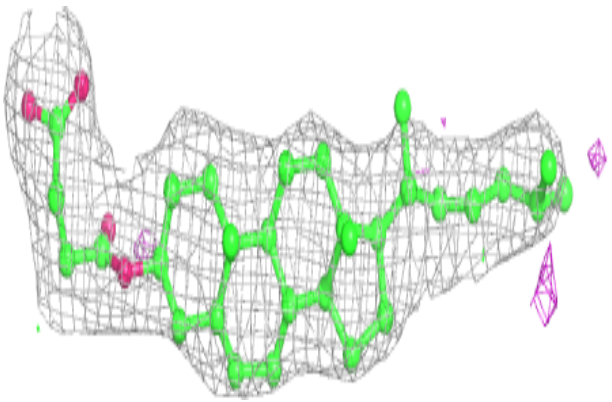


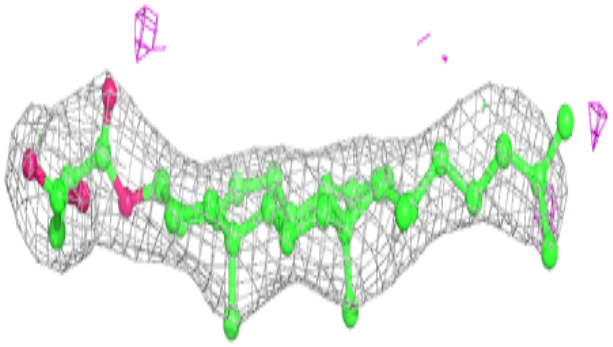


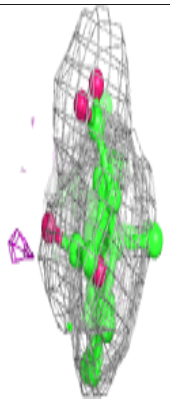


Electron density around Y01 D 303:

$2mF_o$-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.