



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 PM UTC

PDB ID : 5B34 / pdb_00005b34
Title : Serial Femtosecond Crystallography (SFX) of Ground State Bacteriorhodopsin Crystallized from Bicelles in Complex with Iodine-labeled Detergent HAD13a Determined Using 7-keV X-ray Free Electron Laser (XFEL) at SACLA
Authors : Mizohata, E.; Nakane, T.
Deposited on : 2016-02-10
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

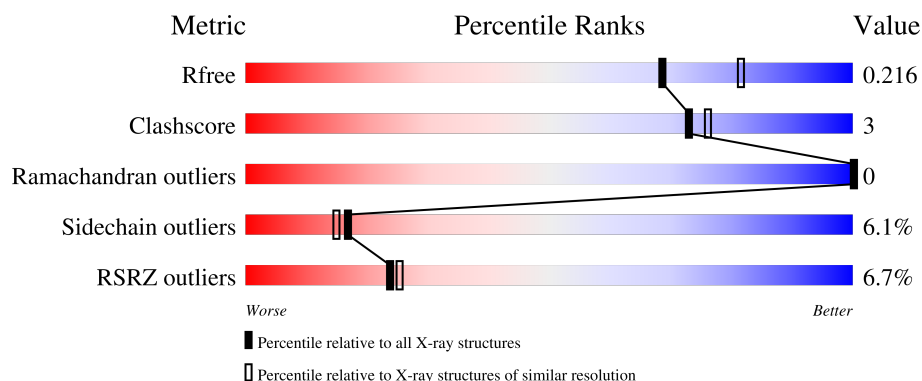
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	249	 6% 80% 9% • 10%

2 Entry composition [i](#)

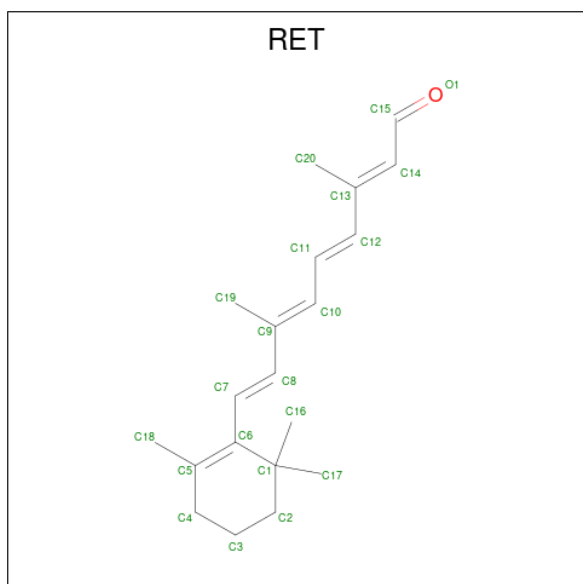
There are 10 unique types of molecules in this entry. The entry contains 1997 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bacteriorhodopsin.

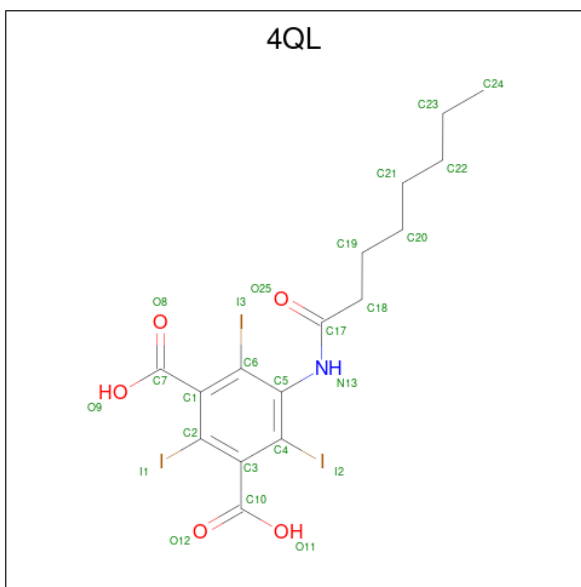
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1741	1172	265	295	9			

- Molecule 2 is RETINAL (CCD ID: RET) (formula: C₂₀H₂₈O).



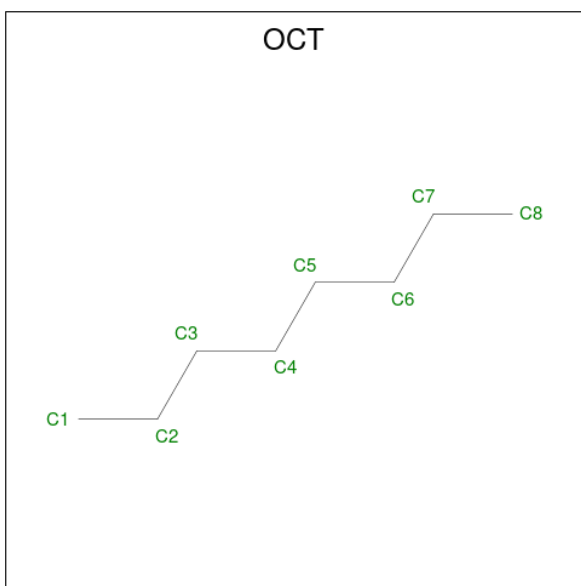
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

- Molecule 3 is 2,4,6-tris(iodanyl)-5-(octanoylamino)benzene-1,3-dicarboxylic acid (CCD ID: 4QL) (formula: C₁₆H₁₈I₃NO₅).



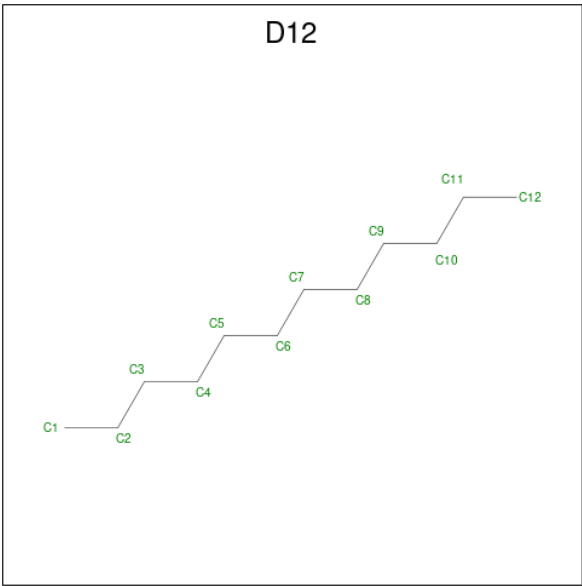
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	I	N	O	0	1
			25	16	3	1	5		
3	A	1	Total	C	I	N	O	0	1
			25	16	3	1	5		

- Molecule 4 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



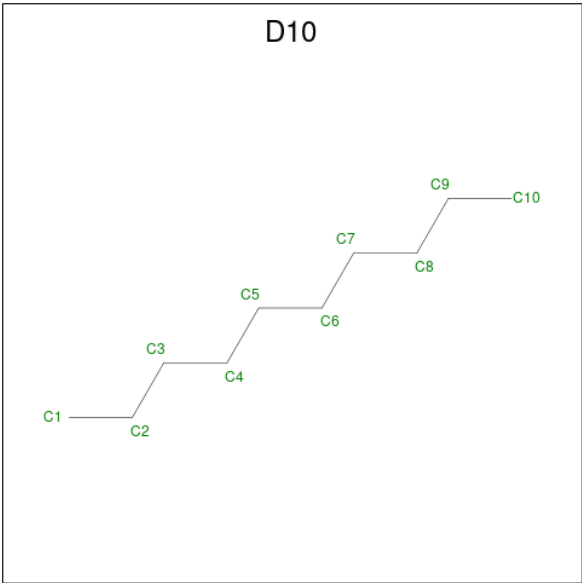
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	1
			8	8		
4	A	1	Total	C	0	1
			8	8		

- Molecule 5 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



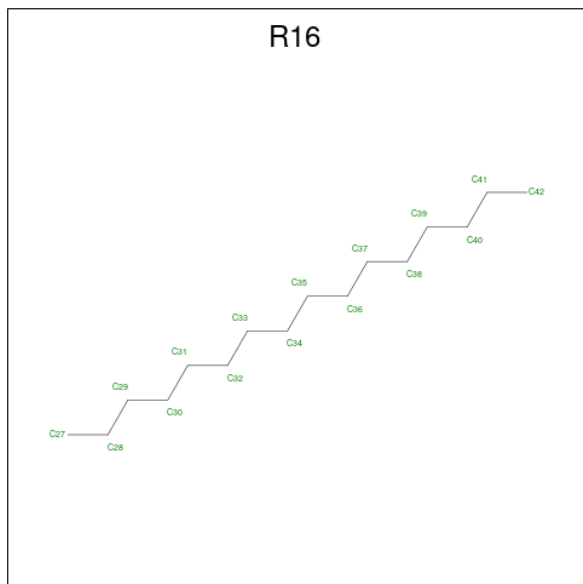
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 12 12	0	0
5	A	1	Total C 12 12	0	0
5	A	1	Total C 12 12	0	0
5	A	1	Total C 12 12	0	0

- Molecule 6 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



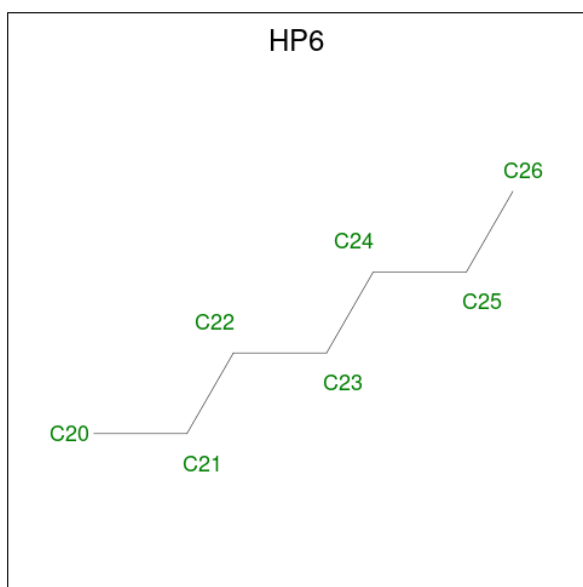
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 10 10	0	0
6	A	1	Total C 10 10	0	0
6	A	1	Total C 10 10	0	0

- Molecule 7 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$).



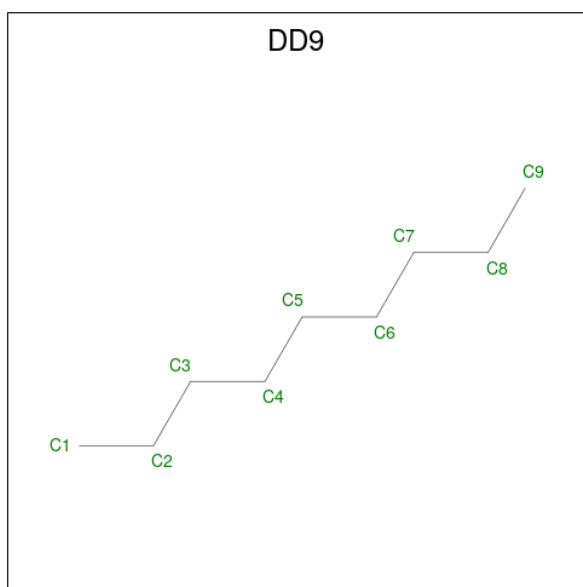
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 16 16	0	0

- Molecule 8 is HEPTANE (CCD ID: HP6) (formula: C_7H_{16}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 7 7	0	0
8	A	1	Total C 7 7	0	0
8	A	1	Total C 7 7	0	0

- Molecule 9 is nonane (CCD ID: DD9) (formula: C_9H_{20}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C 9 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	C	0	0
			9	9		

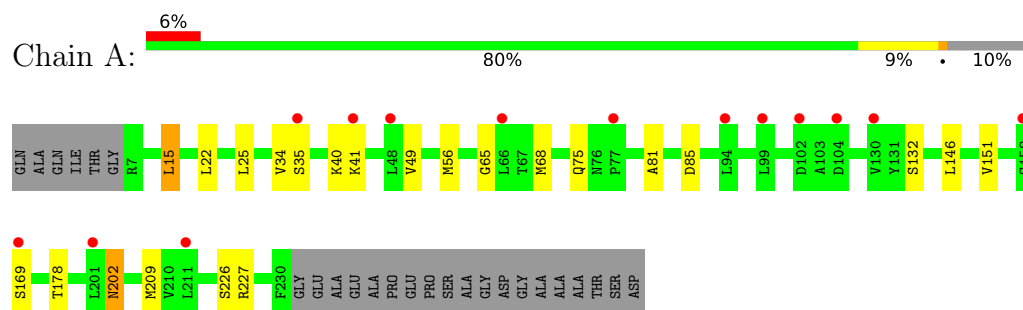
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	37	Total	O	0	0
			37	37		

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: Bacteriorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	46.20Å 103.00Å 128.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.10) 100.0 (50.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.163 , 0.216 0.172 , 0.216	Depositor DCC
R_{free} test set	882 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 129.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1997	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HP6, OCT, DD9, R16, 4QL, D10, D12, RET

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	1.16	1/1789 (0.1%)	1.14	3/2444 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	THR	C-O	-5.54	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ASN	N-CA-C	5.31	116.75	111.07
1	A	49	VAL	CA-C-N	-5.03	114.48	119.56
1	A	49	VAL	C-N-CA	-5.03	114.48	119.56

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	1741	0	1800	8	0
2	A	20	0	27	3	0
3	A	50	0	0	2	0
4	A	16	0	36	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	48	0	104	2	0
6	A	30	0	66	0	0
7	A	16	0	34	0	0
8	A	21	0	48	0	0
9	A	18	0	40	0	0
10	A	37	0	0	1	0
All	All	1997	0	2155	13	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 3.

All (13) 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:A:163:MET:HE3	10:A:421:HOH:O	2.05	0.56
5:A:317:D12:H13	5:A:317:D12:H52	1.89	0.54
2:A:301:RET:H171	2:A:301:RET:H8	1.93	0.51
1:A:15:LEU:HB3	1:A:209:MET:HE2	1.93	0.50
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.95	0.48
1:A:226:SER:HB3	3:A:303[A]:4QL:I3	2.85	0.46
2:A:301:RET:H8	2:A:301:RET:H161	1.96	0.46
1:A:56:MET:HG3	1:A:85:ASP:HB2	1.98	0.45
1:A:68:MET:HB3	1:A:75:GLN:HG3	1.98	0.45
2:A:301:RET:H181	2:A:301:RET:H7	1.76	0.44
1:A:151:VAL:HG22	5:A:306:D12:H22	2.00	0.44
1:A:34:VAL:O	1:A:40:LYS:HE3	2.18	0.43
3:A:302[A]:4QL:O8	3:A:302[A]:4QL:I3	3.07	0.42

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	222/249 (89%)	221 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/195 (93%)	170 (94%)	11 (6%)	17	15

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	22	LEU
1	A	25	LEU
1	A	35	SER
1	A	41	LYS
1	A	132	SER
1	A	146	LEU
1	A	159	LYS
1	A	169	SER
1	A	202	ASN
1	A	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	4QL	A	302[A]	-	25,25,25	1.10	2 (8%)	34,34,34	2.20	9 (26%)
5	D12	A	315	-	11,11,11	0.39	0	10,10,10	0.44	0
5	D12	A	306	-	11,11,11	0.48	0	10,10,10	0.29	0
3	4QL	A	303[A]	-	25,25,25	1.22	3 (12%)	34,34,34	2.29	10 (29%)
8	HP6	A	313	-	6,6,6	0.37	0	5,5,5	0.17	0
4	OCT	A	304[B]	-	7,7,7	0.14	0	6,6,6	0.64	0
2	RET	A	301	1	20,20,21	1.76	5 (25%)	27,27,28	2.16	10 (37%)
4	OCT	A	305[B]	-	7,7,7	0.28	0	6,6,6	0.36	0
5	D12	A	316	-	11,11,11	0.28	0	10,10,10	0.80	1 (10%)
8	HP6	A	312	-	6,6,6	0.32	0	5,5,5	0.42	0
7	R16	A	309	-	15,15,15	0.28	0	14,14,14	0.68	0
9	DD9	A	318	-	8,8,8	0.46	0	7,7,7	0.31	0
5	D12	A	317	-	11,11,11	0.33	0	10,10,10	0.46	0
8	HP6	A	311	-	6,6,6	0.31	0	5,5,5	0.30	0
6	D10	A	310	-	9,9,9	0.43	0	8,8,8	0.27	0
6	D10	A	308	-	9,9,9	0.45	0	8,8,8	0.17	0
9	DD9	A	314	-	8,8,8	0.33	0	7,7,7	0.59	0
6	D10	A	307	-	9,9,9	0.41	0	8,8,8	0.39	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	4QL	A	302[A]	-	-	6/19/19/19	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	D12	A	315	-	-	3/9/9/9	-
5	D12	A	306	-	-	6/9/9/9	-
3	4QL	A	303[A]	-	-	6/19/19/19	0/1/1/1
8	HP6	A	313	-	-	3/4/4/4	-
4	OCT	A	304[B]	-	-	3/5/5/5	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
4	OCT	A	305[B]	-	-	2/5/5/5	-
5	D12	A	316	-	-	4/9/9/9	-
8	HP6	A	312	-	-	1/4/4/4	-
7	R16	A	309	-	-	8/13/13/13	-
9	DD9	A	318	-	-	3/6/6/6	-
5	D12	A	317	-	-	5/9/9/9	-
8	HP6	A	311	-	-	2/4/4/4	-
6	D10	A	310	-	-	4/7/7/7	-
6	D10	A	308	-	-	6/7/7/7	-
9	DD9	A	314	-	-	2/6/6/6	-
6	D10	A	307	-	-	5/7/7/7	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RET	C15-C14	-4.60	1.32	1.49
3	A	303[A]	4QL	C5-N13	-3.94	1.36	1.43
2	A	301	RET	C14-C13	-3.76	1.31	1.33
3	A	302[A]	4QL	C5-N13	-3.49	1.37	1.43
2	A	301	RET	C5-C6	2.59	1.38	1.34
3	A	303[A]	4QL	C5-C4	-2.52	1.36	1.40
2	A	301	RET	C11-C12	-2.34	1.28	1.34
3	A	303[A]	4QL	O9-C7	-2.18	1.24	1.30
2	A	301	RET	C17-C1	2.17	1.57	1.53
3	A	302[A]	4QL	O9-C7	-2.11	1.24	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302[A]	4QL	C4-C5-N13	6.66	125.85	120.63
3	A	302[A]	4QL	C6-C5-N13	-6.25	115.73	120.63
3	A	303[A]	4QL	C6-C1-C7	5.63	125.66	120.30
3	A	303[A]	4QL	C2-C1-C7	-5.21	115.34	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RET	C12-C13-C14	-5.18	104.79	118.55
3	A	303[A]	4QL	C4-C5-N13	-4.94	116.76	120.63
2	A	301	RET	C20-C13-C12	4.85	125.49	118.09
3	A	303[A]	4QL	C18-C17-N13	4.46	122.34	114.59
2	A	301	RET	C7-C8-C9	-4.13	120.12	126.23
3	A	303[A]	4QL	C6-C5-N13	3.82	123.62	120.63
3	A	302[A]	4QL	O11-C10-C3	3.55	124.67	114.67
3	A	302[A]	4QL	C2-C1-C7	3.39	123.52	120.30
3	A	302[A]	4QL	C6-C1-C7	-3.35	117.11	120.30
3	A	302[A]	4QL	O12-C10-C3	-3.22	113.48	121.18
2	A	301	RET	C11-C10-C9	-3.12	122.90	127.28
2	A	301	RET	C10-C11-C12	-3.11	114.19	123.20
3	A	303[A]	4QL	C1-C6-I3	2.81	123.17	119.18
3	A	303[A]	4QL	O25-C17-C18	-2.79	116.97	122.02
3	A	302[A]	4QL	O25-C17-N13	2.60	128.30	123.64
2	A	301	RET	C7-C6-C5	-2.56	115.66	121.56
2	A	301	RET	C19-C9-C8	2.52	121.93	118.09
3	A	302[A]	4QL	C4-C5-C6	-2.28	116.58	118.66
3	A	303[A]	4QL	O11-C10-C3	2.27	121.06	114.67
2	A	301	RET	C8-C9-C10	-2.27	115.44	119.01
3	A	303[A]	4QL	C5-C6-I3	-2.26	116.94	119.30
3	A	302[A]	4QL	O25-C17-C18	-2.25	117.94	122.02
2	A	301	RET	C20-C13-C14	2.21	129.72	123.63
2	A	301	RET	C16-C1-C2	-2.16	100.67	108.95
3	A	303[A]	4QL	C5-C4-I2	-2.07	117.14	119.30
5	A	316	D12	C7-C6-C5	-2.06	103.94	114.37

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303[A]	4QL	C6-C5-N13-C17
3	A	303[A]	4QL	C4-C5-N13-C17
3	A	303[A]	4QL	N13-C17-C18-C19
3	A	303[A]	4QL	O25-C17-C18-C19
4	A	305[B]	OCT	C3-C4-C5-C6
3	A	302[A]	4QL	C20-C21-C22-C23
6	A	307	D10	C2-C3-C4-C5
6	A	308	D10	C5-C6-C7-C8
8	A	313	HP6	C21-C22-C23-C24
5	A	306	D12	C4-C5-C6-C7
3	A	302[A]	4QL	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	316	D12	C11-C10-C9-C8
5	A	315	D12	C11-C10-C9-C8
5	A	317	D12	C7-C8-C9-C10
5	A	316	D12	C7-C8-C9-C10
6	A	308	D10	C3-C4-C5-C6
6	A	310	D10	C2-C3-C4-C5
9	A	318	DD9	C4-C5-C6-C7
5	A	317	D12	C4-C5-C6-C7
3	A	303[A]	4QL	C20-C21-C22-C23
9	A	318	DD9	C2-C3-C4-C5
6	A	310	D10	C4-C5-C6-C7
6	A	307	D10	C1-C2-C3-C4
5	A	306	D12	C6-C7-C8-C9
9	A	318	DD9	C3-C4-C5-C6
7	A	309	R16	C39-C40-C41-C42
4	A	305[B]	OCT	C1-C2-C3-C4
5	A	306	D12	C2-C3-C4-C5
8	A	311	HP6	C20-C21-C22-C23
4	A	304[B]	OCT	C1-C2-C3-C4
3	A	303[A]	4QL	C21-C22-C23-C24
7	A	309	R16	C34-C35-C36-C37
6	A	307	D10	C3-C4-C5-C6
9	A	314	DD9	C5-C6-C7-C8
3	A	302[A]	4QL	C19-C20-C21-C22
5	A	317	D12	C2-C3-C4-C5
6	A	308	D10	C4-C5-C6-C7
5	A	317	D12	C1-C2-C3-C4
3	A	302[A]	4QL	C2-C1-C7-O8
8	A	311	HP6	C22-C23-C24-C25
8	A	313	HP6	C23-C24-C25-C26
5	A	316	D12	C2-C3-C4-C5
5	A	306	D12	C1-C2-C3-C4
7	A	309	R16	C38-C39-C40-C41
6	A	308	D10	C1-C2-C3-C4
7	A	309	R16	C32-C33-C34-C35
4	A	304[B]	OCT	C5-C6-C7-C8
6	A	308	D10	C6-C7-C8-C9
4	A	304[B]	OCT	C2-C3-C4-C5
6	A	307	D10	C6-C7-C8-C9
7	A	309	R16	C27-C28-C29-C30
3	A	302[A]	4QL	C2-C1-C7-O9
9	A	314	DD9	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	312	HP6	C20-C21-C22-C23
6	A	307	D10	C4-C5-C6-C7
8	A	313	HP6	C22-C23-C24-C25
6	A	310	D10	C7-C8-C9-C10
6	A	310	D10	C3-C4-C5-C6
7	A	309	R16	C33-C34-C35-C36
5	A	306	D12	C9-C10-C11-C12
6	A	308	D10	C7-C8-C9-C10
5	A	315	D12	C1-C2-C3-C4
5	A	316	D12	C6-C7-C8-C9
7	A	309	R16	C30-C31-C32-C33
5	A	306	D12	C5-C6-C7-C8
5	A	317	D12	C3-C4-C5-C6
7	A	309	R16	C29-C30-C31-C32
3	A	302[A]	4QL	C6-C1-C7-O8
5	A	315	D12	C9-C10-C11-C12

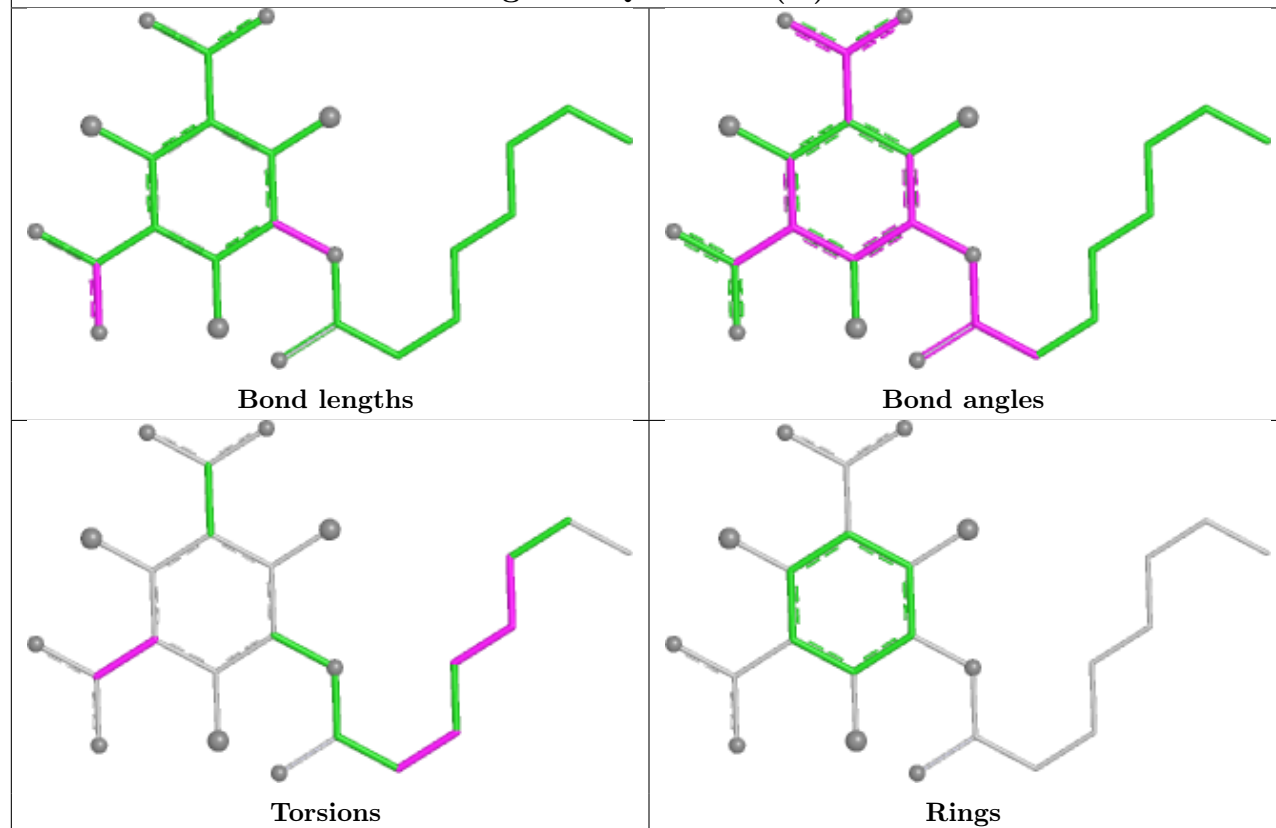
There are no ring outliers.

5 monomers are involved in 7 short contacts:

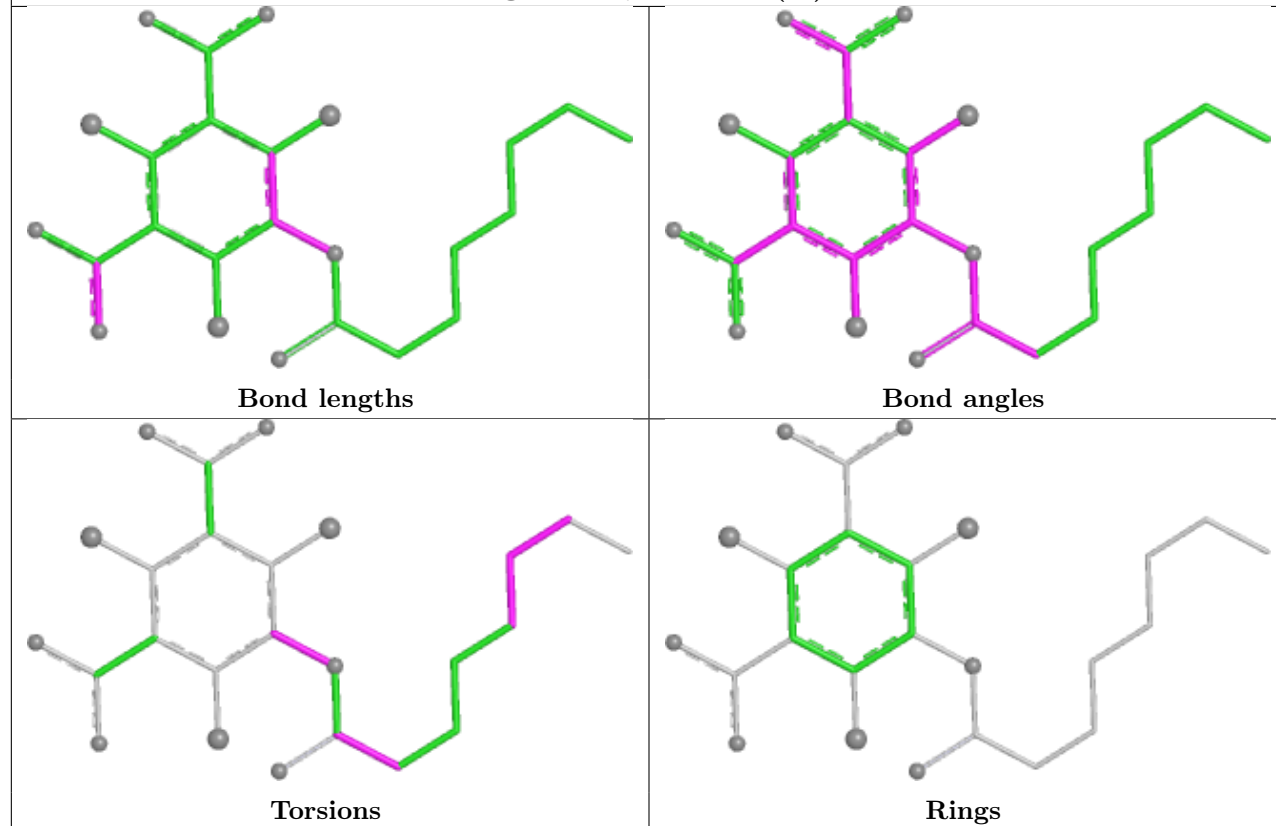
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302[A]	4QL	1	0
5	A	306	D12	1	0
3	A	303[A]	4QL	1	0
2	A	301	RET	3	0
5	A	317	D12	1	0

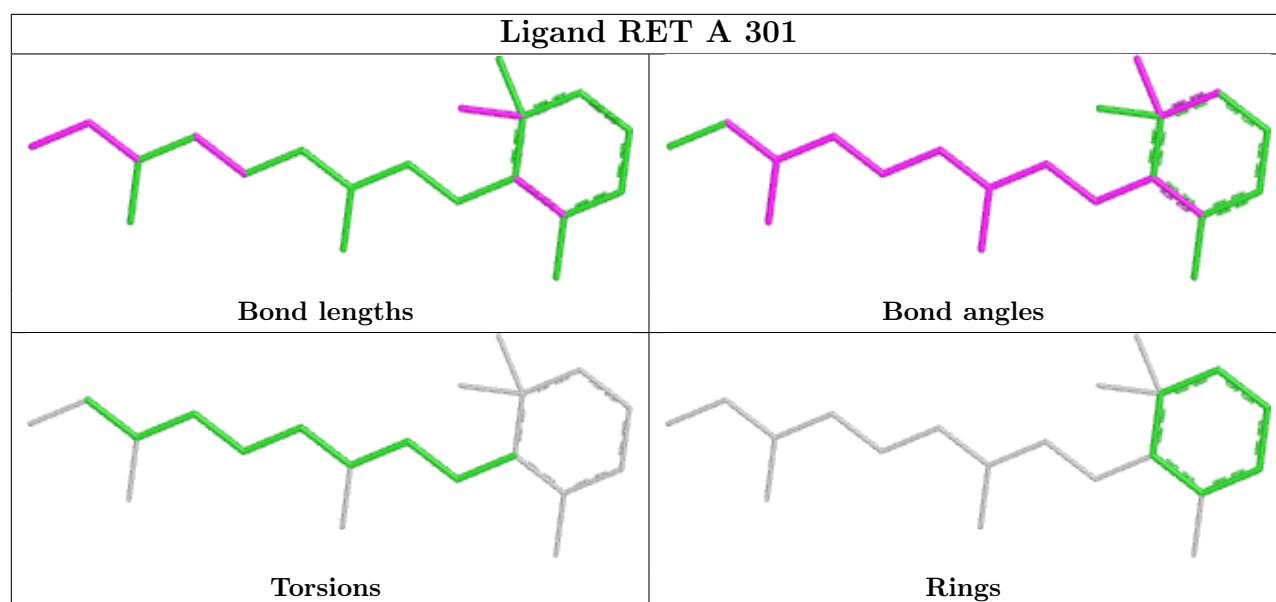
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 4QL A 302 (A)



Ligand 4QL A 303 (A)





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	224/249 (89%)	0.87	15 (6%) 24 25	53, 61, 83, 107	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	VAL	5.5
1	A	168	ALA	2.8
1	A	158	SER	2.7
1	A	35	SER	2.4
1	A	66	LEU	2.4
1	A	99	LEU	2.3
1	A	94	LEU	2.3
1	A	41	LYS	2.3
1	A	102	ASP	2.3
1	A	104	ASP	2.2
1	A	48	LEU	2.2
1	A	77	PRO	2.1
1	A	201	LEU	2.1
1	A	169	SER	2.1
1	A	211	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

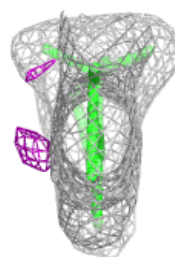
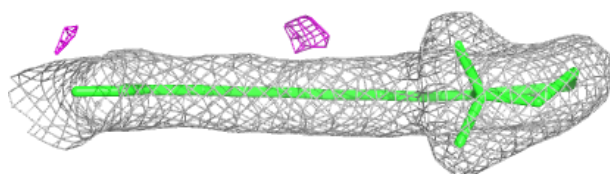
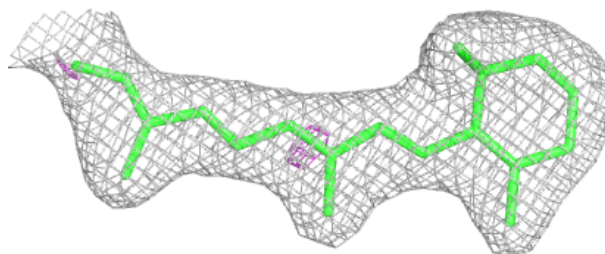
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D10	A	308	10/10	0.70	0.28	97,112,117,121	0
9	DD9	A	318	9/9	0.77	0.29	100,108,119,120	0
8	HP6	A	312	7/7	0.85	0.29	104,107,109,112	0
9	DD9	A	314	9/9	0.87	0.19	102,104,109,111	0
5	D12	A	317	12/12	0.88	0.22	92,99,104,105	0
6	D10	A	307	10/10	0.89	0.22	93,99,101,105	0
6	D10	A	310	10/10	0.89	0.23	92,105,113,120	0
8	HP6	A	311	7/7	0.89	0.19	96,101,102,103	0
5	D12	A	306	12/12	0.90	0.21	72,90,107,111	0
5	D12	A	316	12/12	0.91	0.21	96,101,106,108	0
8	HP6	A	313	7/7	0.91	0.24	73,94,105,107	0
4	OCT	A	305[B]	8/8	0.92	0.25	70,79,82,83	8
7	R16	A	309	16/16	0.93	0.19	67,85,96,108	0
5	D12	A	315	12/12	0.93	0.19	89,96,104,112	0
2	RET	A	301	20/21	0.95	0.11	50,55,64,70	0
3	4QL	A	303[A]	25/25	0.95	0.17	65,84,102,117	25
3	4QL	A	302[A]	25/25	0.96	0.15	64,79,100,114	25
4	OCT	A	304[B]	8/8	0.97	0.15	63,67,70,72	8

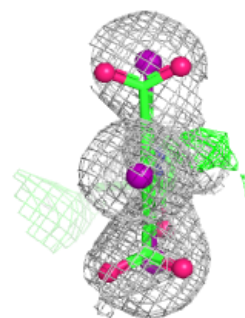
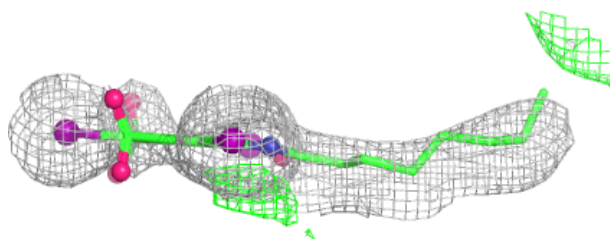
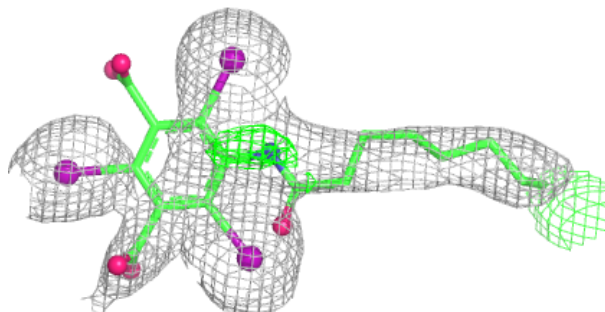
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RET 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)

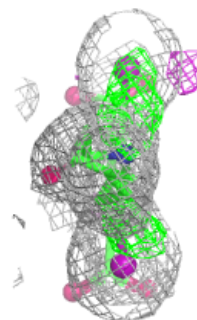
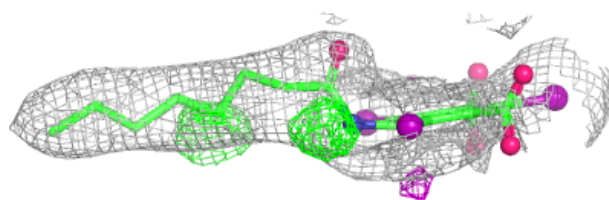
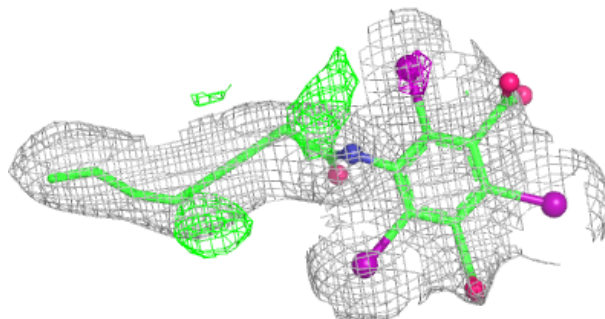
**Electron density around 4QL A 303 (A):**

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



Electron density around 4QL A 302 (A):

$2mF_o-DF_c$ (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.