wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 06:56 PM EST

PDB ID	:	3UVV
Title	:	Crystal Structure of the ligand binding domains of the thyroid receptor:retinoid X receptor complexed with 3,3',5 triiodo-L-thyronine and 9-cis retinoic acid
Authors	:	Fernandez, E.J.; Putcha, B.-D.K.; Wright, E.; Brunzelle, J.S.
Deposited on	:	2011-11-30
Resolution	:	2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

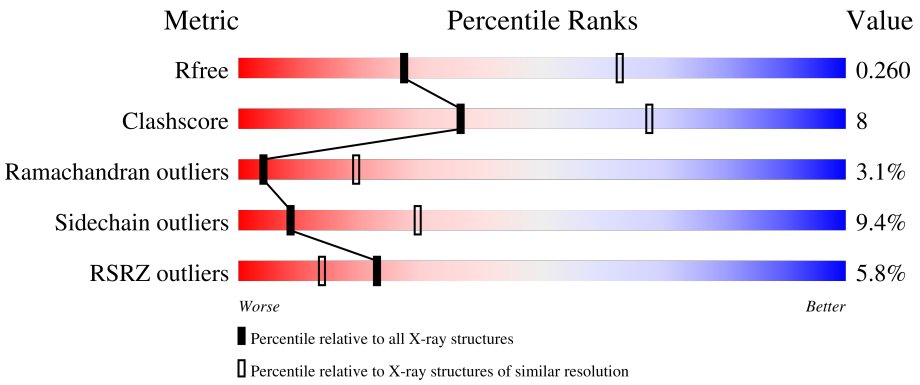
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	265	6% 67% 25% • • 6%
2	B	244	5% 69% 18% • 11%

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	T3	A	501	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3755 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 Thyroid hormone receptor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1971	1263	332	360	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	GLY	-	expression tag	UNP P04625
A	145	SER	-	expression tag	UNP P04625
A	146	HIS	-	expression tag	UNP P04625
A	147	GLU	-	expression tag	UNP P04625

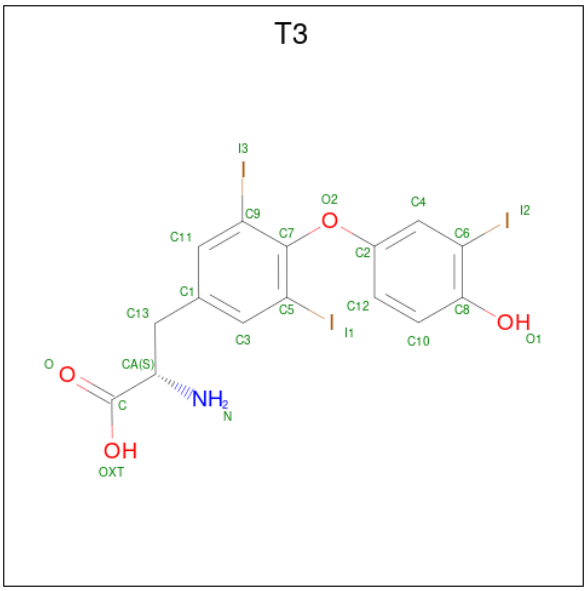
- Molecule 2 is a protein called Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	1720	1103	295	312	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

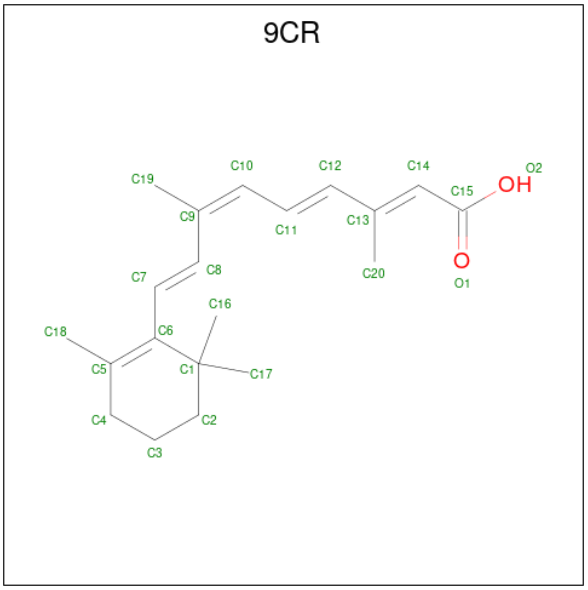
Chain	Residue	Modelled	Actual	Comment	Reference
B	221	MET	-	expression tag	UNP P19793
B	222	LYS	-	expression tag	UNP P19793
B	223	LYS	-	expression tag	UNP P19793
B	224	GLY	-	expression tag	UNP P19793
B	463	MET	-	expression tag	UNP P19793
B	464	THR	-	expression tag	UNP P19793

- Molecule 3 is 3,5,3'TRIIODOTHYRONINE (three-letter code: T3) (formula: $C_{15}H_{12}I_3NO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	I	N	O		
3	A	1	23	15	3	1	4	0	0

- Molecule 4 is (9cis)-retinoic acid (three-letter code: 9CR) (formula: $C_{20}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	22	20	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	11	11	11	0	0
			Total	O		
5	B	8	8	8	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: Thyroid hormone receptor alpha

Chain A: 6% 67% 25% • • 6%

GLY SER HIS E147 M148 I149 K150 Q153 H154 S159 A160 L165 I166 H167 V168 V169 T170 E171 A172 H173 R174 S175 T176 N177 A178 Q179 G180 S181 H182 W183 K184 Q185 K186 R187 K188 F189 L190 P191 E192 D193 I194 GLY GLN SER PRO MET ALA SER MET P203 D204 GLY D206 K207 E215 F216

T217 K218 I219 I220 T221 I224 T225 R226 V227 V228 D229 F230 M236 P241 C242 E243 D244 Q245 I246 E255 R260 Y265 D266 S269 E270 T271 L272 G276 E277 M278 A279 Q284 I297 E313 V314 A315 L321 D326 C332 V333 D334 K335 K338 C339 Q340

E341 T342 Y343 L344 L345 A346 F347 I351 N357 H360 K364 L365 K368 L372 C390 P391 T392 F395 V402 F403 E404 D405 GLN GLU VAL

• Molecule 2: Retinoic acid receptor RXR-alpha

Chain B: 5% 69% 18% • 11%

MET LYS LYS GLY SER ALA N227 E228 D229 M230 P231 V232 E233 R234 E237 P244 K245 T246 GLU THR TYR VAL GLU ALA ASN MET GLY LEU ASN PRO SER SER P261 V265 I268 A271 A272 D273 K274 Q275 L276 F277 T278 L279 V280 L294 L301 R302 L308 S312

V320 K321 D322 G323 I324 L325 L326 A327 T328 G329 L330 H333 R334 N335 V342 E352 M360 Q361 T365 C369 L370 R371 L375 L383 S384 N385 V389 E410 Q411 P412 G413 R414 L419 L420 R421 R426 C432 L433 L436 F439 I442 T445

D448 T449 F450 M454 L455 P458 HIS GLN MET THR MET THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	129.13Å 165.32Å 85.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.55 – 2.95 27.32 – 2.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (27.55-2.95) 98.9 (27.32-2.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.94Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.201 , 0.250 0.211 , 0.260	Depositor DCC
R_{free} test set	952 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	97.4	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 95.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3755	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: T3, 9CR

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	0.51	0/2012	0.79	4/2719 (0.1%)
2	B	0.51	0/1755	0.70	0/2374
All	All	0.51	0/3767	0.75	4/5093 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	391	PRO	N-CA-C	7.35	131.20	112.10
1	A	391	PRO	CA-N-CD	-6.35	102.61	111.50
1	A	203	PRO	N-CA-CB	6.05	110.56	103.30
1	A	390	CYS	CA-C-N	5.61	132.82	117.10

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	1971	0	1960	39	0
2	B	1720	0	1755	22	0
3	A	23	0	5	7	0
4	B	22	0	27	6	0
5	A	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	8	0	0	0	0
All	All	3755	0	3747	59	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 8.

The worst 5 of 59 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:169:VAL:HG21	1:A:343:TYR:HE2	1.30	0.93
2:B:320:VAL:HG21	2:B:325:LEU:HB2	1.63	0.77
1:A:219:ILE:HD11	3:A:501:T3:I1	2.57	0.75
1:A:220:ILE:CD1	3:A:501:T3:I1	3.11	0.69
1:A:176:THR:HG21	1:A:230:PHE:HB2	1.75	0.68

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	244/265 (92%)	215 (88%)	18 (7%)	11 (4%)	2 12
2	B	214/244 (88%)	197 (92%)	14 (6%)	3 (1%)	11 39
All	All	458/509 (90%)	412 (90%)	32 (7%)	14 (3%)	4 19

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	MET
1	A	160	ALA
1	A	192	GLU

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Mol	Chain	Res	Type
1	A	390	CYS
1	A	391	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	216/236 (92%)	197 (91%)	19 (9%)	10 33
2	B	188/210 (90%)	169 (90%)	19 (10%)	7 26
All	All	404/446 (91%)	366 (91%)	38 (9%)	8 29

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	361	GLN
2	B	433	LEU
2	B	365	THR
2	B	419	LEU
2	B	450	PHE

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

Mol	Chain	Res	Type
2	B	297	GLN
2	B	385	ASN
2	B	435	HIS
2	B	411	GLN
1	A	245	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	T3	A	501	-	23,24,24	1.33	3 (13%)	33,34,34	1.05	2 (6%)
4	9CR	B	501	-	22,22,22	1.13	2 (9%)	30,30,30	2.19	10 (33%)

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	T3	A	501	-	-	3/12/12/12	0/2/2/2
4	9CR	B	501	-	-	4/15/32/32	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	T3	C8-C6	4.42	1.48	1.39
3	A	501	T3	C7-C5	2.52	1.48	1.40
4	B	501	9CR	C12-C13	-2.30	1.41	1.45
3	A	501	T3	C7-C9	2.28	1.47	1.40
4	B	501	9CR	C1-C6	2.17	1.56	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	9CR	C19-C9-C10	-6.18	114.26	122.92
4	B	501	9CR	C16-C1-C6	5.07	118.53	110.30
4	B	501	9CR	C7-C8-C9	-3.15	121.47	126.23
4	B	501	9CR	C19-C9-C8	2.91	122.66	118.08
4	B	501	9CR	C8-C9-C10	2.69	123.06	118.94

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	T3	C1-C13-CA-N
4	B	501	9CR	C1-C6-C7-C8
4	B	501	9CR	C5-C6-C7-C8
3	A	501	T3	OXT-C-CA-C13
3	A	501	T3	O-C-CA-C13

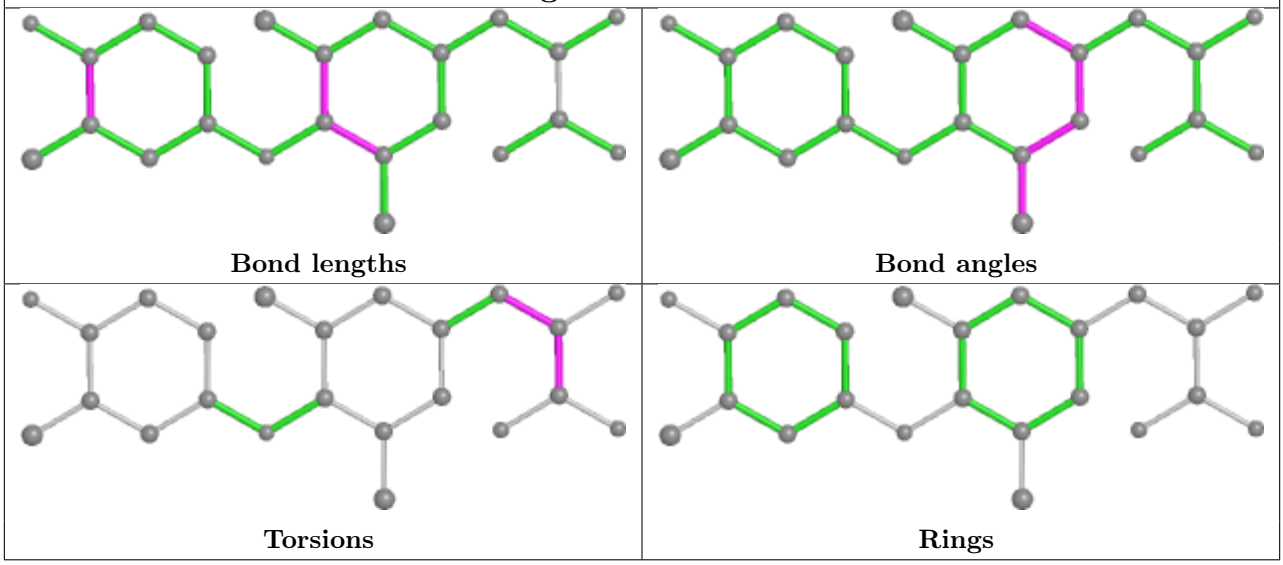
There are no ring outliers.

2 monomers are involved in 13 short contacts:

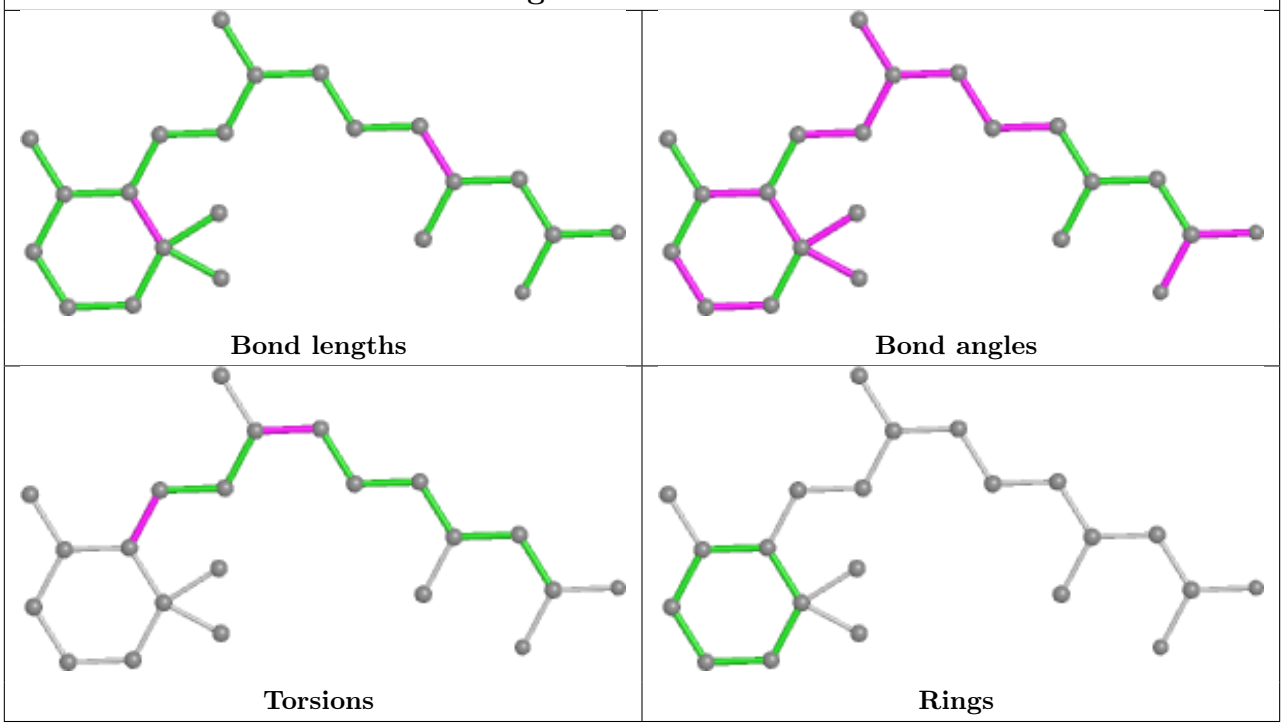
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	T3	7	0
4	B	501	9CR	6	0

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 T3 A 501



Ligand 9CR B 501



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	250/265 (94%)	0.28	15 (6%)	21	13	85, 114, 170, 195	8 (3%)
2	B	218/244 (89%)	0.25	12 (5%)	25	15	80, 110, 143, 173	0
All	All	468/509 (91%)	0.27	27 (5%)	23	14	80, 112, 146, 195	8 (1%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	TRP	5.8
1	A	182	HIS	5.6
2	B	261	PRO	5.0
1	A	185	GLN	4.5
1	A	181	SER	4.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

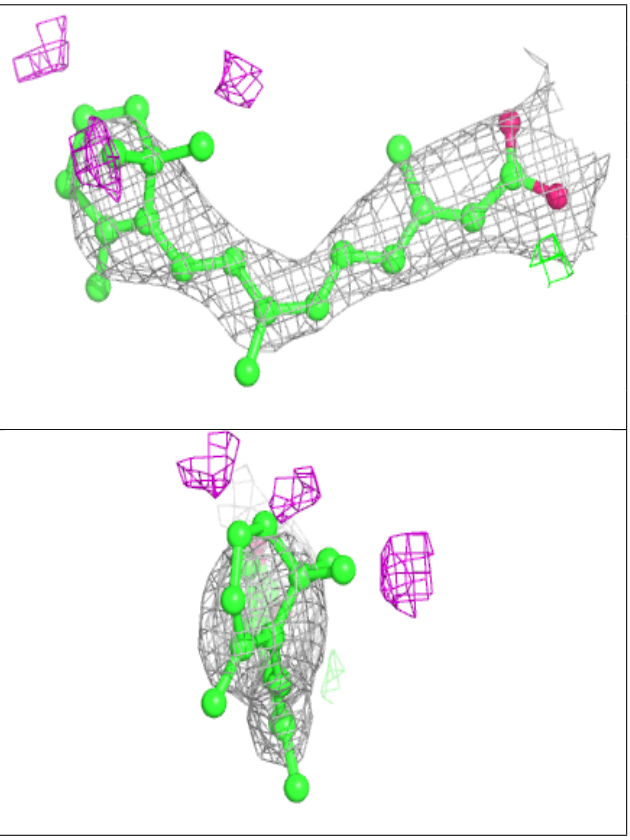
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	9CR	B	501	22/22	0.84	0.37	89,99,111,112	0
3	T3	A	501	23/23	0.97	0.35	88,98,109,121	23

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.

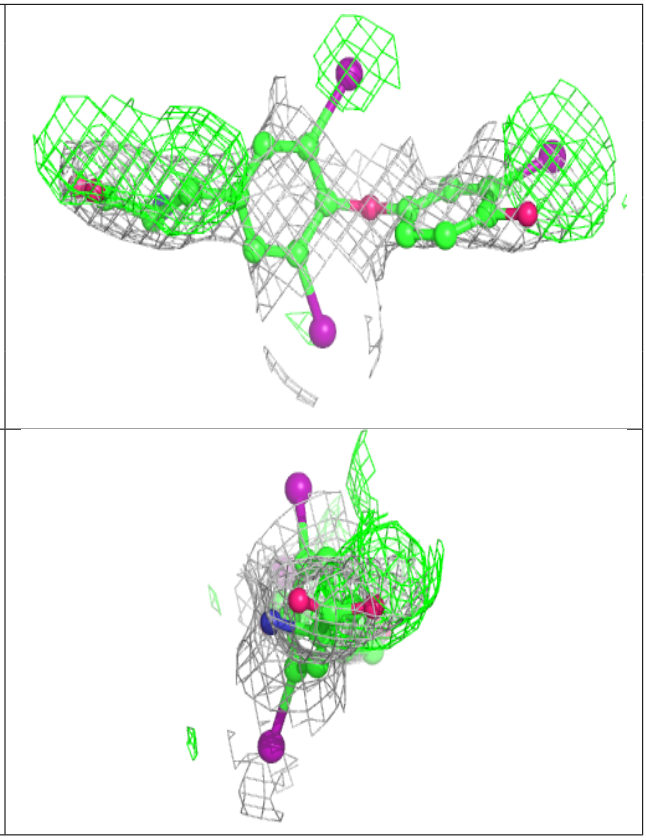
Electron density around 9CR B 501:

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 T3 A 501:

$2mF_o$-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.