



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:45 PM UTC

PDB ID : 3UVV / pdb_00003uvv
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 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

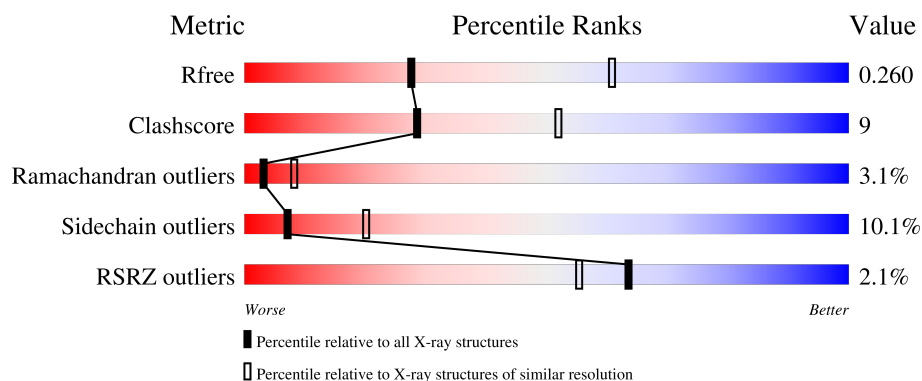
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

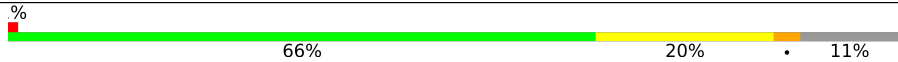
The reported resolution of this entry is 2.95 Å.

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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	265	
2	B	244	

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

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
1	A	250	Total	C	N	O	S	0	0	0
			1971	1263	332	360	16			

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

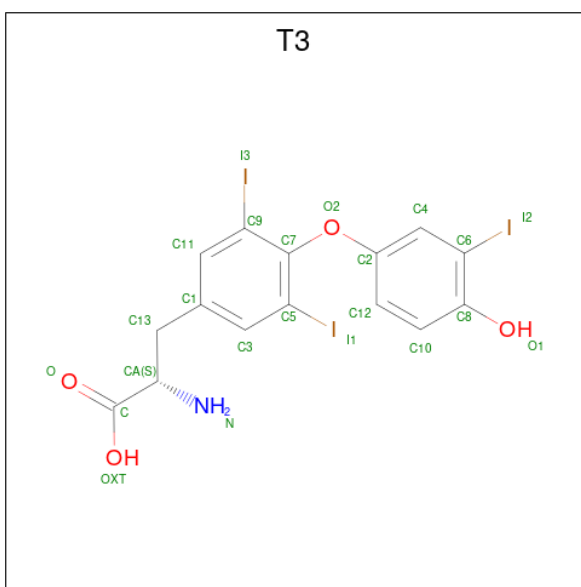
- Molecule 2 is a protein called Retinoic acid receptor RXR-alpha.

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

There are 6 discrepancies between the modelled and reference sequences:

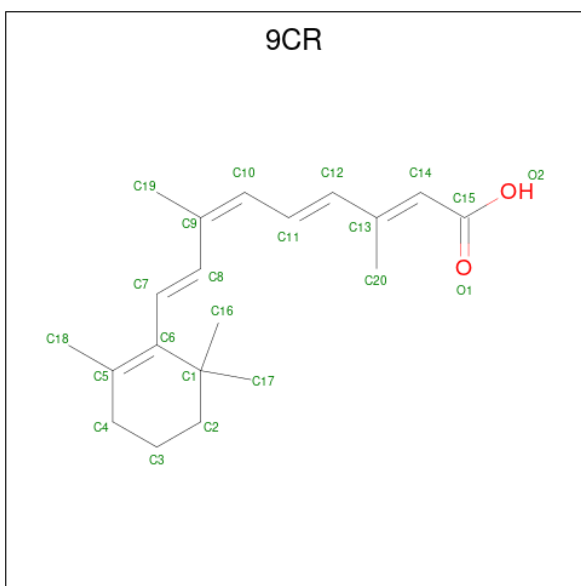
Chain	Residue	Modelled	Actual	Comment	Reference
B	221	MET	-	expression tag	UNP P19793
B	222	LYS	-	expression tag	UNP P19793
B	223	LYS	-	expression tag	UNP P19793
B	224	GLY	-	expression tag	UNP P19793
B	463	MET	-	expression tag	UNP P19793
B	464	THR	-	expression tag	UNP P19793

- Molecule 3 is 3,5,3'TRIIODOTHYRONINE (CCD ID: T3) (formula: C₁₅H₁₂I₃NO₄).



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

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



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

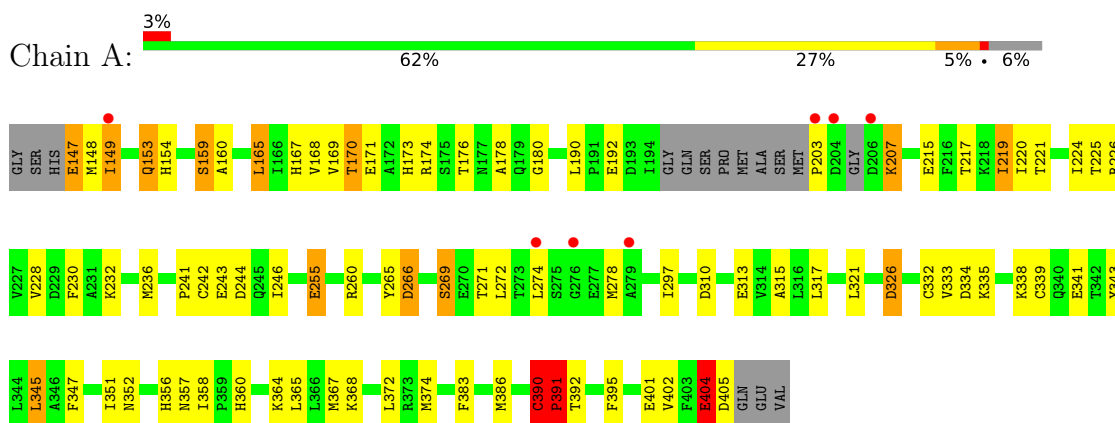
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	8	Total 8	O 8	0	0

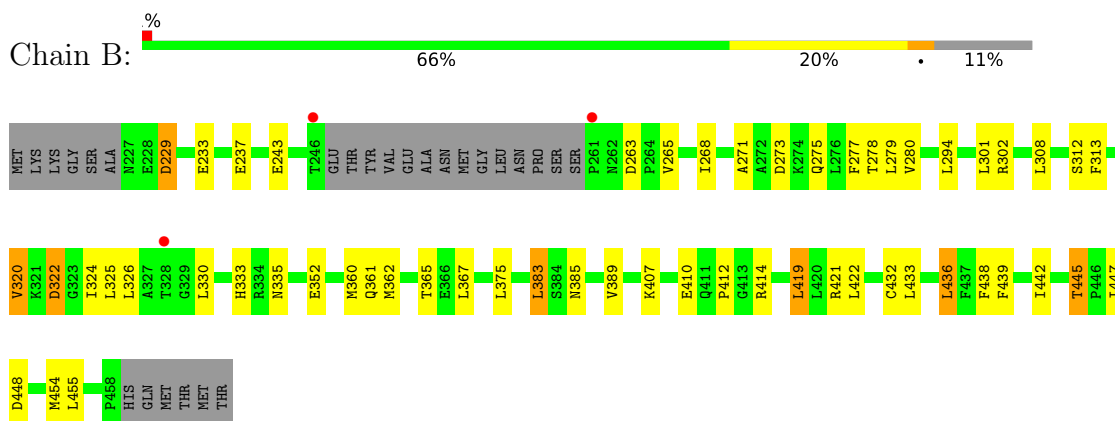
3 Residue-property plots

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



• Molecule 2: Retinoic acid receptor RXR-alpha



4 Data and refinement statistics

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 27.55 – 2.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (27.55-2.95) 98.7 (27.55-2.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 89.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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

5.1 Standard geometry

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

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	0.88	2/2012 (0.1%)	1.57	25/2719 (0.9%)
2	B	0.87	0/1755	1.52	6/2374 (0.3%)
All	All	0.88	2/3767 (0.1%)	1.55	31/5093 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	GLN	CA-C	5.71	1.59	1.53
1	A	374	MET	SD-CE	5.50	1.93	1.79

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	PRO	N-CA-C	7.35	131.20	112.10
1	A	203	PRO	N-CA-CB	6.88	110.56	103.00
2	B	229	ASP	N-CA-C	-6.85	104.50	112.92
1	A	317	LEU	CA-C-N	6.74	129.21	120.44
1	A	317	LEU	C-N-CA	6.74	129.21	120.44
1	A	390	CYS	CA-C-O	-6.70	110.98	120.16
1	A	347	PHE	CA-CB-CG	6.47	120.27	113.80
1	A	391	PRO	CA-N-CD	-6.35	102.61	111.50
2	B	438	PHE	CA-CB-CG	6.31	120.11	113.80
2	B	263	ASP	CA-CB-CG	6.13	118.73	112.60
2	B	445	THR	CB-CA-C	5.93	117.92	109.38
1	A	153	GLN	CA-C-N	5.75	133.34	123.05
1	A	153	GLN	C-N-CA	5.75	133.34	123.05
1	A	390	CYS	CA-C-N	5.60	140.44	127.00
1	A	390	CYS	C-N-CA	5.60	140.44	127.00
1	A	168	VAL	N-CA-CB	5.58	117.07	110.55
2	B	313	PHE	CA-CB-CG	5.52	119.32	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	SER	CA-C-N	5.42	131.89	121.54
1	A	159	SER	C-N-CA	5.42	131.89	121.54
1	A	326	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	232	LYS	CA-C-N	5.32	127.95	120.28
1	A	232	LYS	C-N-CA	5.32	127.95	120.28
2	B	243	GLU	N-CA-C	5.26	117.04	109.04
1	A	310	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	352	ASN	CA-C-N	5.10	127.11	120.28
1	A	352	ASN	C-N-CA	5.10	127.11	120.28
1	A	404	GLU	CA-C-N	5.04	130.77	121.70
1	A	404	GLU	C-N-CA	5.04	130.77	121.70
1	A	401	GLU	CA-C-N	5.04	127.01	120.56
1	A	401	GLU	C-N-CA	5.04	127.01	120.56
1	A	266	ASP	CB-CA-C	5.03	115.94	110.15

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	1971	0	1960	44	0
2	B	1720	0	1755	26	0
3	A	23	0	5	7	0
4	B	22	0	27	6	0
5	A	11	0	0	0	0
5	B	8	0	0	0	0
All	All	3755	0	3747	66	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 9.

All (66) 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
2:B:360:MET:O	2:B:414:ARG:NH2	2.27	0.66
1:A:269:SER:HB2	1:A:271:THR:HG22	1.78	0.66
2:B:302:ARG:HA	2:B:454:MET:HE1	1.77	0.65
1:A:220:ILE:HD13	3:A:501:T3:I1	2.67	0.65
1:A:220:ILE:HD12	3:A:501:T3:I1	2.68	0.63
1:A:169:VAL:HG21	1:A:343:TYR:CE2	2.23	0.62
1:A:147:GLU:O	1:A:149:ILE:N	2.32	0.61
1:A:326:ASP:HB2	2:B:352:GLU:HG2	1.82	0.61
1:A:367:MET:HE3	2:B:419:LEU:HD13	1.84	0.60
1:A:219:ILE:CD1	3:A:501:T3:I1	3.20	0.60
1:A:297:ILE:HD13	3:A:501:T3:I3	2.72	0.59
2:B:432:CYS:SG	4:B:501:9CR:H16	2.43	0.58
2:B:279:LEU:HD11	2:B:308:LEU:HD13	1.87	0.56
1:A:220:ILE:HB	3:A:501:T3:I1	2.76	0.55
1:A:167:HIS:HA	1:A:170:THR:HG22	1.88	0.55
2:B:280:VAL:HG12	2:B:301:LEU:HD13	1.89	0.53
1:A:390:CYS:HB3	1:A:391:PRO:O	2.08	0.53
1:A:367:MET:HE1	2:B:422:LEU:HD12	1.91	0.53
1:A:241:PRO:HD2	1:A:332:CYS:SG	2.50	0.52
1:A:274:LEU:HD12	1:A:278:MET:HE3	1.92	0.51
1:A:224:ILE:HG21	1:A:402:VAL:HG21	1.92	0.51
1:A:345:LEU:HD11	2:B:412:PRO:HB2	1.93	0.51
1:A:332:CYS:HB3	1:A:335:LYS:HB2	1.93	0.50
2:B:362:MET:HE3	2:B:367:LEU:HB2	1.93	0.50
2:B:275:GLN:HG3	4:B:501:9CR:O2	2.12	0.49
1:A:392:THR:HA	1:A:395:PHE:HD1	1.77	0.49
2:B:273:ASP:CG	2:B:448:ASP:HB3	2.38	0.49
2:B:436:LEU:HD22	2:B:455:LEU:HD11	1.95	0.49
2:B:439:PHE:HA	2:B:442:ILE:HG12	1.95	0.48
1:A:217:THR:HA	1:A:220:ILE:HG22	1.95	0.48
1:A:255:GLU:HB3	1:A:321:LEU:HD13	1.96	0.48
2:B:302:ARG:HA	2:B:454:MET:CE	2.42	0.48
1:A:169:VAL:CG2	1:A:343:TYR:HE2	2.16	0.47
1:A:224:ILE:O	1:A:228:VAL:HG23	2.15	0.47
2:B:410:GLU:O	2:B:412:PRO:HD3	2.15	0.47
1:A:265:TYR:HB2	1:A:272:LEU:HD23	1.96	0.47
1:A:365:LEU:O	1:A:368:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:ASP:HB3	2:B:333:HIS:CE1	2.50	0.46
1:A:236:MET:HB2	1:A:339:CYS:SG	2.55	0.46
2:B:268:ILE:HD13	4:B:501:9CR:H1	1.98	0.46
2:B:265:VAL:HG12	2:B:445:THR:HG21	1.97	0.46
1:A:169:VAL:HG12	1:A:315:ALA:HB1	2.00	0.44
1:A:171:GLU:HA	1:A:174:ARG:HB2	1.99	0.44
1:A:190:LEU:HD11	1:A:215:GLU:HG3	1.99	0.44
1:A:241:PRO:HG2	1:A:244:ASP:HB2	2.00	0.44
2:B:268:ILE:HG23	4:B:501:9CR:H27	2.00	0.44
2:B:383:LEU:HD22	2:B:389:VAL:HG21	1.99	0.44
1:A:321:LEU:HD11	1:A:372:LEU:HD13	2.00	0.43
1:A:383:PHE:HA	1:A:386:MET:HE2	2.00	0.43
1:A:404:GLU:O	1:A:405:ASP:HB2	2.17	0.43
1:A:176:THR:HG23	1:A:226:ARG:HB3	2.00	0.43
1:A:356:HIS:C	1:A:358:ILE:H	2.27	0.42
1:A:165:LEU:O	1:A:169:VAL:HG23	2.19	0.42
1:A:338:LYS:HA	1:A:341:GLU:HB2	2.02	0.42
2:B:436:LEU:HD11	4:B:501:9CR:H23	2.01	0.42
1:A:360:HIS:O	1:A:364:LYS:HB2	2.19	0.42
1:A:173:HIS:HD2	1:A:260:ARG:HH21	1.66	0.41
2:B:277:PHE:O	2:B:280:VAL:HG22	2.20	0.41
1:A:176:THR:HG22	1:A:260:ARG:NH2	2.36	0.41
2:B:271:ALA:HB2	2:B:326:LEU:HD23	2.03	0.41
2:B:436:LEU:HG	4:B:501:9CR:C18	2.50	0.41

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 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	214/244 (88%)	197 (92%)	14 (6%)	3 (1%)	9	24
All	All	458/509 (90%)	412 (90%)	32 (7%)	14 (3%)	3	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	MET
1	A	160	ALA
1	A	192	GLU
1	A	390	CYS
1	A	391	PRO
2	B	320	VAL
1	A	159	SER
1	A	333	VAL
1	A	207	LYS
2	B	322	ASP
1	A	178	ALA
1	A	357	ASN
2	B	385	ASN
1	A	180	GLY

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	216/236 (92%)	194 (90%)	22 (10%)	7	20
2	B	188/210 (90%)	169 (90%)	19 (10%)	7	20
All	All	404/446 (91%)	363 (90%)	41 (10%)	7	20

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	GLU
1	A	149	ILE

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Mol	Chain	Res	Type
1	A	153	GLN
1	A	154	HIS
1	A	165	LEU
1	A	170	THR
1	A	207	LYS
1	A	219	ILE
1	A	221	THR
1	A	225	THR
1	A	242	CYS
1	A	243	GLU
1	A	246	ILE
1	A	255	GLU
1	A	266	ASP
1	A	269	SER
1	A	313	GLU
1	A	334	ASP
1	A	345	LEU
1	A	351	ILE
1	A	391	PRO
1	A	404	GLU
2	B	229	ASP
2	B	233	GLU
2	B	237	GLU
2	B	278	THR
2	B	294	LEU
2	B	312	SER
2	B	324	ILE
2	B	330	LEU
2	B	335	ASN
2	B	361	GLN
2	B	365	THR
2	B	375	LEU
2	B	383	LEU
2	B	407	LYS
2	B	419	LEU
2	B	421	ARG
2	B	433	LEU
2	B	436	LEU
2	B	447	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
1	A	167	HIS
1	A	173	HIS
1	A	179	GLN
1	A	318	GLN
1	A	340	GLN
1	A	352	ASN
2	B	297	GLN
2	B	377	ASN
2	B	411	GLN
2	B	435	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	9CR	B	501	-	22,22,22	1.14	2 (9%)	30,30,30	2.16	11 (36%)
3	T3	A	501	-	23,24,24	1.37	3 (13%)	30,34,34	1.07	2 (6%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	T3	C8-C6	4.60	1.48	1.39
3	A	501	T3	C7-C5	2.60	1.48	1.40
3	A	501	T3	C7-C9	2.35	1.47	1.40
4	B	501	9CR	C12-C13	-2.31	1.41	1.46
4	B	501	9CR	C1-C6	2.31	1.56	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	9CR	C16-C1-C6	5.28	118.53	110.24
4	B	501	9CR	C19-C9-C10	-5.28	114.26	122.82
4	B	501	9CR	C7-C8-C9	-3.22	121.47	126.23
4	B	501	9CR	C19-C9-C8	2.99	122.66	118.09
4	B	501	9CR	C17-C1-C16	-2.63	101.12	108.63
4	B	501	9CR	C8-C9-C10	2.58	123.06	119.01
4	B	501	9CR	O2-C15-O1	-2.41	117.80	122.70
4	B	501	9CR	C1-C6-C5	-2.40	119.35	122.64
4	B	501	9CR	C2-C3-C4	2.36	116.46	111.28
4	B	501	9CR	C10-C11-C12	-2.25	116.69	123.20
3	A	501	T3	C3-C5-I1	2.15	122.50	118.46
4	B	501	9CR	C1-C6-C7	2.02	121.12	115.65
3	A	501	T3	C11-C1-C3	2.00	121.73	119.01

There are no chirality outliers.

All (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

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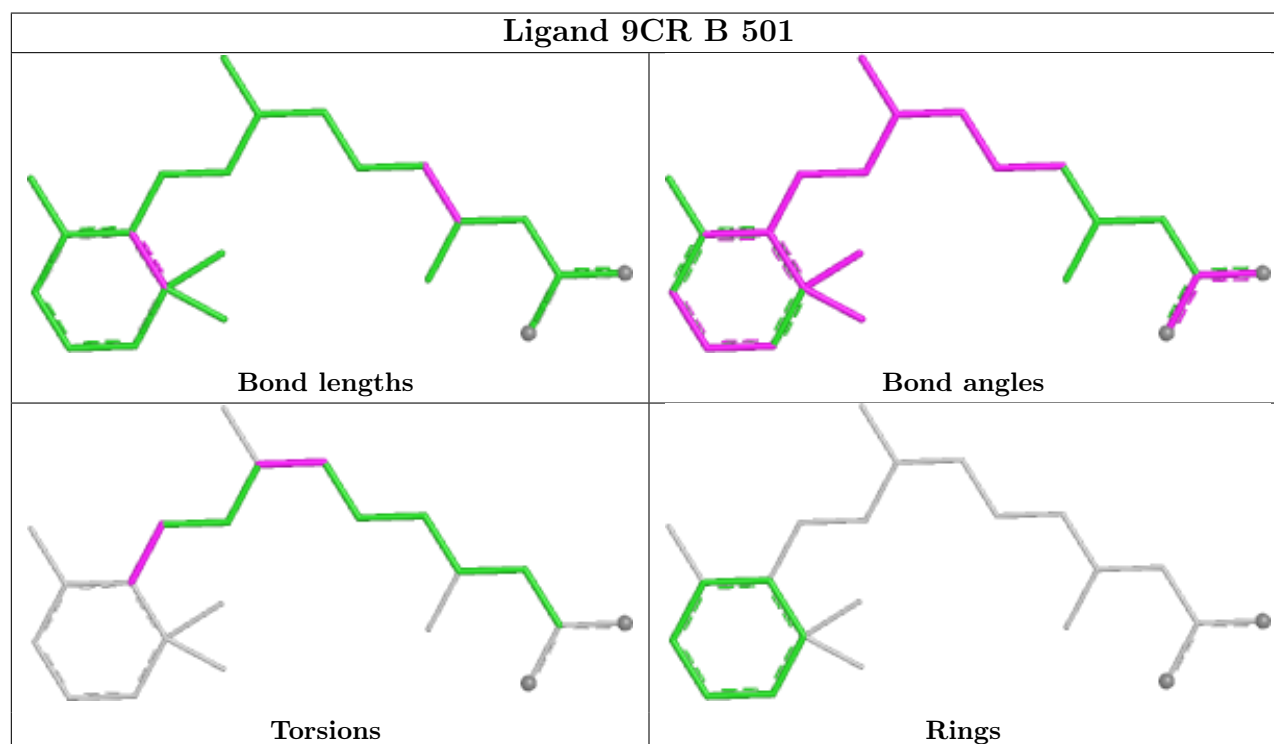
Mol	Chain	Res	Type	Atoms
3	A	501	T3	O-C-CA-C13
4	B	501	9CR	C11-C10-C9-C19
4	B	501	9CR	C11-C10-C9-C8

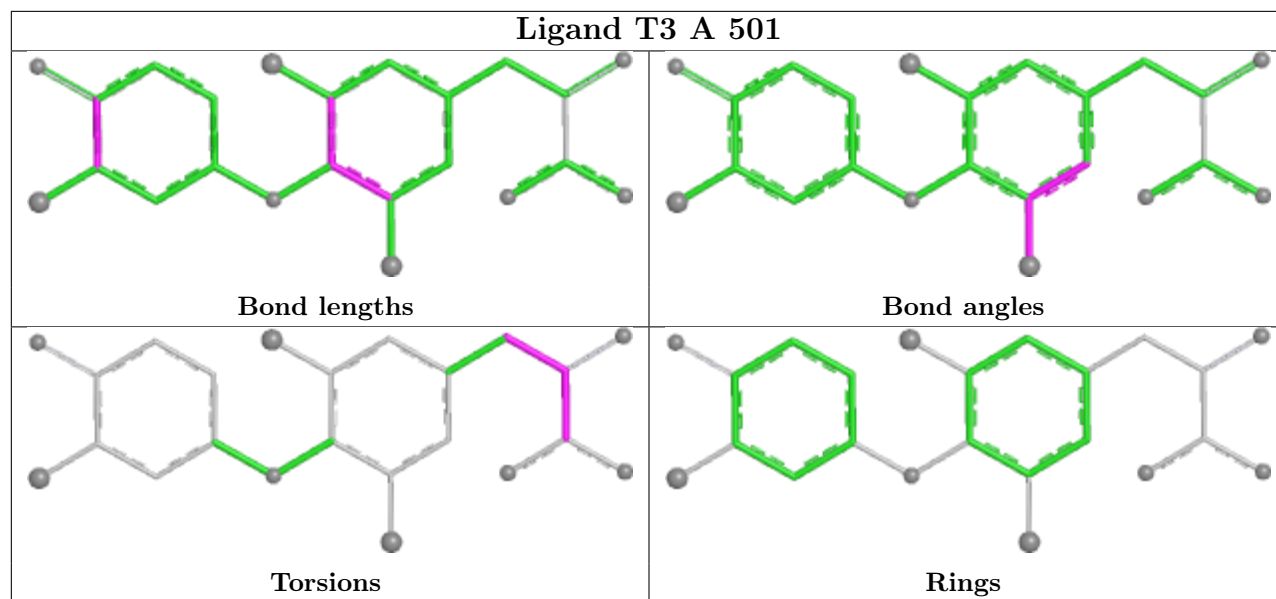
There are no ring outliers.

2 monomers are involved in 13 short contacts:

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





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%)	0.16	7 (2%) 55 47	84, 112, 170, 195	8 (3%)
2	B	218/244 (89%)	-0.12	3 (1%) 73 67	80, 110, 143, 173	0
All	All	468/509 (91%)	0.03	10 (2%) 63 55	80, 111, 146, 195	8 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ASP	4.9
1	A	203	PRO	2.4
1	A	274	LEU	2.3
1	A	276	GLY	2.2
1	A	206	ASP	2.2
2	B	328	THR	2.1
1	A	149	ILE	2.1
2	B	261	PRO	2.1
2	B	246	THR	2.1
1	A	279	ALA	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 ⓘ

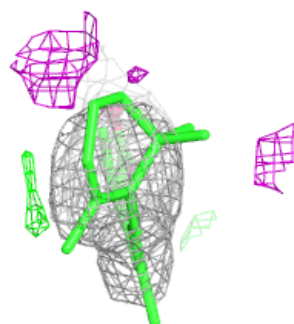
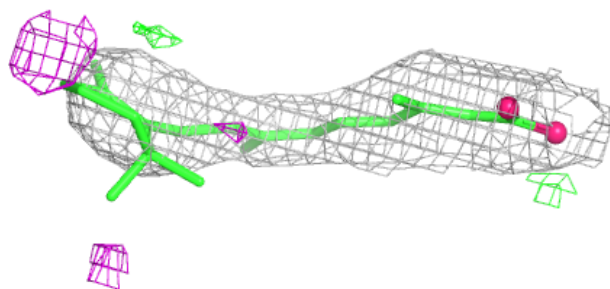
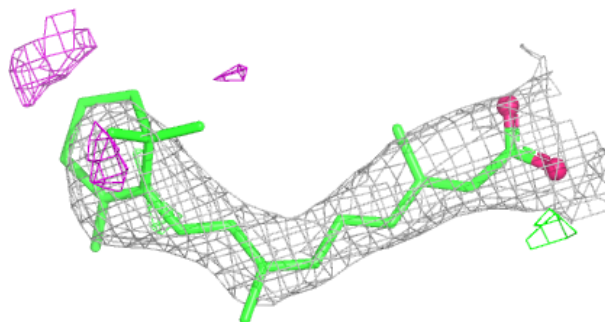
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

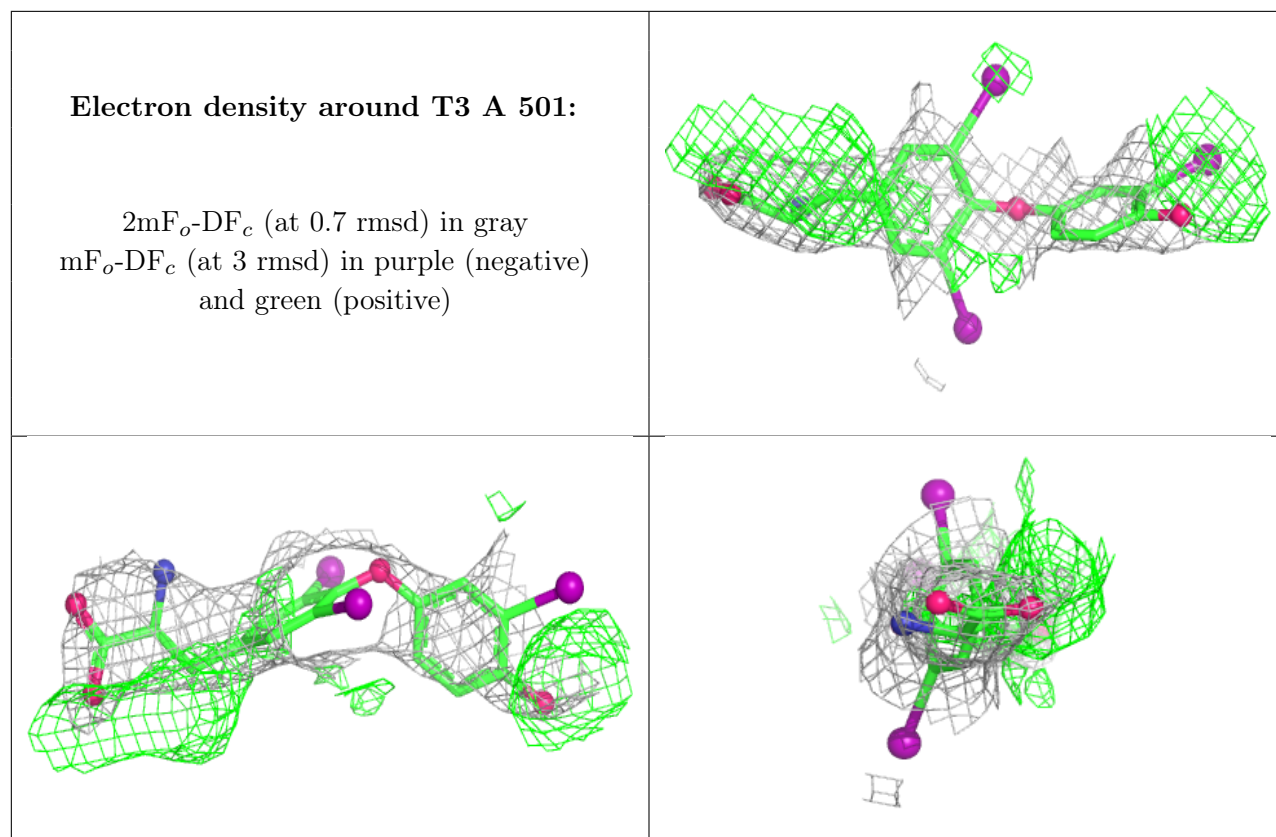
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	9CR	B	501	22/22	0.96	0.15	89,99,111,112	0
3	T3	A	501	23/23	0.98	0.11	88,98,109,121	23

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.