



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:45 AM UTC

PDB ID : 1Y0X / pdb_00001y0x
Title : Thyroxine-Thyroid Hormone Receptor Interactions
Authors : Sandler, B.; Webb, P.; Apriletti, J.W.; Huber, B.R.; Togashi, M.; Cunha Lima, S.T.; Juric, S.; Nilsson, S.; Wagner, R.; Fletterick, R.J.; Baxter, J.D.
Deposited on : 2004-11-16
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	:	4-5-2 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

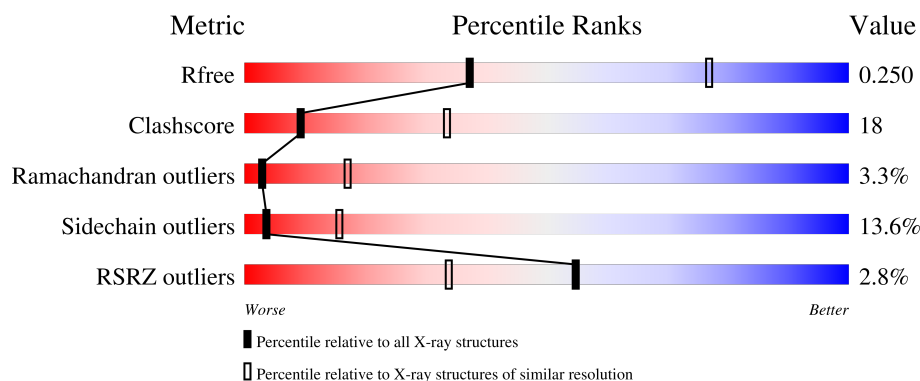
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. 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	X	281	2% 35% 38% 14% • 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
2	CAC	X	503	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	T44	X	500	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1974 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.

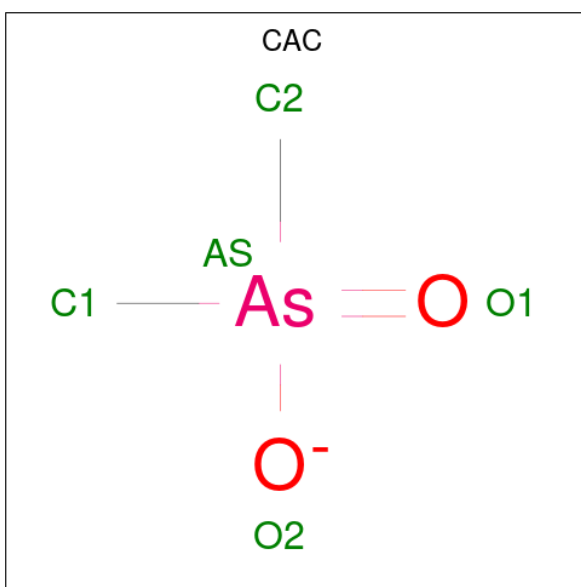
- Molecule 1 is a protein called Thyroid hormone receptor beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	250	Total	C	N	O	S	0	0	0
			1934	1243	325	350	16			

There are 21 discrepancies between the modelled and reference sequences:

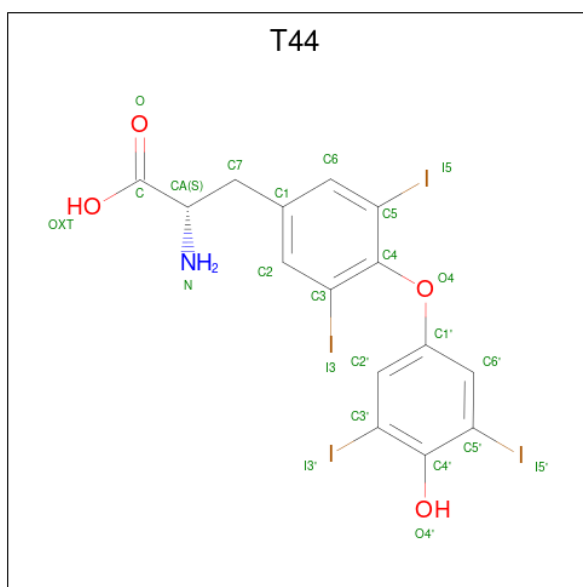
Chain	Residue	Modelled	Actual	Comment	Reference
X	181	MET	-	expression tag	UNP P10828
X	182	GLY	-	expression tag	UNP P10828
X	183	SER	-	expression tag	UNP P10828
X	184	SER	-	expression tag	UNP P10828
X	185	HIS	-	expression tag	UNP P10828
X	186	HIS	-	expression tag	UNP P10828
X	187	HIS	-	expression tag	UNP P10828
X	188	HIS	-	expression tag	UNP P10828
X	189	HIS	-	expression tag	UNP P10828
X	190	HIS	-	expression tag	UNP P10828
X	191	SER	-	expression tag	UNP P10828
X	192	SER	-	expression tag	UNP P10828
X	193	GLY	-	expression tag	UNP P10828
X	194	LEU	-	expression tag	UNP P10828
X	195	VAL	-	expression tag	UNP P10828
X	196	PRO	-	expression tag	UNP P10828
X	197	ARG	-	expression tag	UNP P10828
X	198	GLY	-	expression tag	UNP P10828
X	199	SER	-	expression tag	UNP P10828
X	200	HIS	-	expression tag	UNP P10828
X	201	MET	-	expression tag	UNP P10828

- Molecule 2 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total 1	As 1	0	0
2	X	1	Total 1	As 1	0	0
2	X	1	Total 1	As 1	0	0
2	X	1	Total 1	As 1	0	0
2	X	1	Total 1	As 1	0	0
2	X	1	Total 1	As 1	0	0

- Molecule 3 is 3,5,3',5'-TETRAIODO-L-THYRONINE (CCD ID: T44) (formula: C₁₅H₁₁I₄NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	X	1	Total	C	I	N	O	0
			24	15	4	1	4	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	10	Total	O	0	0
			10	10		

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.

Chain X:

2% 35% 38% 14% 11%

Category	Value
MET	2%
GLY	35%
SER	38%
GLN	14%
ALA	11%
PRO	2%
ILE	2%
VAL	2%
ASN	2%
ASP	2%
THR	2%
LEU	2%
ARG	2%
GLY	2%
SER	2%
GLN	2%
ALA	2%
PRO	2%
ILE	2%
VAL	2%
ASN	2%
ASP	2%
THR	2%
LEU	2%
ARG	2%
GLY	2%
SER	2%
GLN	2%
ALA	2%
PRO	2%
ILE	2%
VAL	2%
ASN	2%
ASP	2%
THR	2%
LEU	2%
ARG	2%
GLY	2%
SER	2%
GLN	2%
ALA	2%
PRO	2%
ILE	2%
VAL	2%
ASN	2%
ASP	2%
THR	2%
LEU	2%
ARG	2%
GLY	2%
SER	2%
GLN	2%
ALA	2%
PRO	2%
ILE	2%
VAL	2%
ASN	2%
ASP	2%
THR	2%
LEU	2%
ARG	2%
GLY	2%
SER	2%
GLN	2%
ALA	2%
PRO	2%
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ASN	2%
ASP	2%
THR	2%
LEU	2%
ARG	2%
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SER	2%
GLN	2%
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PRO	2%
ILE	2%
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ASP	2%
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ARG	2%
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SER	2%
GLN	2%
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PRO	2%
ILE	2%
VAL	2%
ASN	2%
ASP	2%
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ARG	2%
GLY	2%
SER	2%
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ALA	2%
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SER	2%
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VAL	2%
ASN	2%
ASP	2%
THR	2%
LEU	2%
ARG	2%
GLY	2%
SER	2%
GLN	2%
ALA	2%
PRO	2%
ILE	2%
VAL	2%
ASN	2%
ASP	2%
THR	2%
LEU	2%
ARG	2%
GLY	2%
SER	2%
GLN	2%
ALA	2%
PRO	2%
ILE	2%
VAL	2%
ASN	2%
ASP	2%
THR	2%
LEU	2%
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SER	2%
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GLY	2%
SER	2%
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ALA	2%
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GLY	2%
SER	2%
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GLY	2%
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SER	2%
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GLY	2%
SER	2%
GLN	2%
ALA	2%
PRO	2%
ILE	2%
VAL	2%
ASN	2%
ASP	2%
THR	2%
LEU	2%
ARG	2%
GLY	2%
SER	2%
GLN	2%

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	68.79Å 68.79Å 130.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.76 – 3.10 59.57 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (59.76-3.10) 99.7 (59.57-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.266 0.206 , 0.250	Depositor DCC
R_{free} test set	960 reflections (10.44%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1974	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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: T44, CAC

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	X	2.37	81/1977 (4.1%)	1.83	37/2681 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	449	GLU	CA-CB	9.54	1.68	1.53
1	X	223	LYS	CA-CB	9.52	1.68	1.53
1	X	392	ILE	CA-CB	-9.07	1.43	1.54
1	X	433	ALA	CA-CB	-8.94	1.39	1.53
1	X	250	ILE	CA-CB	-8.75	1.43	1.54
1	X	275	ILE	C-O	-8.63	1.14	1.24
1	X	217	GLU	CA-CB	8.52	1.66	1.53
1	X	393	GLU	C-O	-8.43	1.14	1.24
1	X	458	VAL	C-O	-8.37	1.14	1.24
1	X	393	GLU	CA-C	-8.35	1.42	1.52
1	X	312	ILE	CA-CB	-8.34	1.44	1.54
1	X	217	GLU	CA-C	8.18	1.63	1.52
1	X	438	ARG	NE-CZ	-7.97	1.24	1.33
1	X	219	TRP	CA-C	-7.86	1.42	1.52
1	X	208	ILE	C-O	7.54	1.33	1.24
1	X	233	ASN	N-CA	-7.38	1.36	1.46
1	X	319	VAL	CA-CB	-7.27	1.44	1.54
1	X	220	GLU	CA-C	6.92	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	205	GLN	CA-C	6.91	1.62	1.52
1	X	274	LYS	CA-CB	6.79	1.63	1.53
1	X	308	CYS	CA-C	-6.72	1.43	1.52
1	X	346	LEU	C-O	-6.71	1.15	1.24
1	X	387	ALA	CA-CB	6.71	1.64	1.53
1	X	431	ILE	CA-CB	6.71	1.62	1.54
1	X	459	PHE	CA-C	6.68	1.61	1.52
1	X	441	HIS	CB-CG	6.54	1.59	1.50
1	X	414	VAL	CA-CB	-6.52	1.46	1.54
1	X	379	MET	SD-CE	-6.48	1.63	1.79
1	X	313	MET	CA-C	-6.45	1.44	1.52
1	X	375	ALA	C-O	6.44	1.31	1.24
1	X	333	GLU	N-CA	6.44	1.54	1.46
1	X	330	LEU	C-O	-6.37	1.16	1.23
1	X	250	ILE	CA-C	6.30	1.59	1.52
1	X	430	MET	SD-CE	-6.26	1.64	1.79
1	X	456	LEU	CA-C	-6.24	1.44	1.52
1	X	293	PHE	CA-C	-6.22	1.44	1.52
1	X	448	THR	N-CA	6.22	1.54	1.46
1	X	283	VAL	C-O	-6.14	1.16	1.24
1	X	271	HIS	CA-C	6.10	1.60	1.52
1	X	207	SER	CA-CB	-6.06	1.45	1.53
1	X	367	ASP	C-O	-6.03	1.16	1.24
1	X	318	ALA	C-O	6.01	1.31	1.24
1	X	336	VAL	CA-CB	-6.00	1.45	1.54
1	X	414	VAL	CA-C	-5.92	1.45	1.52
1	X	314	SER	CA-C	-5.92	1.45	1.52
1	X	238	HIS	CA-C	5.90	1.61	1.52
1	X	391	ARG	NE-CZ	-5.89	1.26	1.33
1	X	333	GLU	CA-C	5.87	1.60	1.52
1	X	384	PRO	C-O	5.85	1.30	1.23
1	X	287	ALA	C-O	-5.79	1.17	1.24
1	X	336	VAL	CA-C	-5.71	1.45	1.52
1	X	237	SER	N-CA	5.71	1.53	1.46
1	X	313	MET	SD-CE	5.63	1.93	1.79
1	X	351	ASP	N-CA	-5.61	1.39	1.46
1	X	329	THR	CA-C	-5.61	1.45	1.52
1	X	238	HIS	CA-CB	5.60	1.62	1.53
1	X	417	PHE	CA-C	5.59	1.59	1.52
1	X	383	ARG	CA-C	-5.59	1.46	1.53
1	X	333	GLU	C-O	-5.58	1.17	1.24
1	X	388	CYS	CA-C	5.55	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	445	GLU	N-CA	5.50	1.53	1.46
1	X	220	GLU	CD-OE2	5.41	1.35	1.25
1	X	420	LYS	CA-C	-5.40	1.45	1.52
1	X	230	VAL	N-CA	5.38	1.52	1.46
1	X	328	LEU	CA-C	-5.38	1.46	1.52
1	X	404	GLU	CA-C	-5.37	1.46	1.52
1	X	304	LEU	C-O	-5.36	1.17	1.24
1	X	301	GLN	CD-OE1	-5.35	1.13	1.23
1	X	371	ALA	N-CA	-5.30	1.39	1.46
1	X	342	LYS	CA-C	5.30	1.59	1.52
1	X	233	ASN	CA-C	5.29	1.58	1.53
1	X	396	GLN	CD-OE1	-5.22	1.13	1.23
1	X	225	VAL	CA-CB	-5.17	1.48	1.54
1	X	452	PRO	CA-CB	-5.15	1.47	1.54
1	X	281	THR	CA-CB	5.14	1.61	1.53
1	X	296	LEU	CA-CB	5.10	1.61	1.53
1	X	267	GLU	CA-CB	5.09	1.61	1.53
1	X	447	PRO	CA-C	-5.06	1.46	1.52
1	X	276	ILE	CG1-CD1	-5.03	1.32	1.51
1	X	434	CYS	CA-CB	5.03	1.61	1.53
1	X	290	LEU	C-O	-5.03	1.18	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	413	HIS	CA-CB-CG	-9.18	104.62	113.80
1	X	207	SER	N-CA-C	-8.90	102.93	113.88
1	X	455	PHE	N-CA-C	-8.02	102.49	111.07
1	X	419	PRO	CA-N-CD	-7.35	101.71	112.00
1	X	447	PRO	CB-CA-C	-7.23	102.71	111.46
1	X	324	GLU	N-CA-C	-7.18	103.15	110.97
1	X	334	MET	N-CA-C	7.12	120.50	108.90
1	X	267	GLU	N-CA-C	-6.93	103.66	111.14
1	X	201	MET	N-CA-C	-6.89	104.69	113.23
1	X	447	PRO	CA-C-O	-6.76	113.32	121.03
1	X	363	PHE	CA-C-N	-6.50	113.03	122.19
1	X	363	PHE	C-N-CA	-6.50	113.03	122.19
1	X	201	MET	CA-C-N	6.28	133.53	121.54
1	X	201	MET	C-N-CA	6.28	133.53	121.54
1	X	281	THR	OG1-CB-CG2	-6.12	97.07	109.30
1	X	216	ASP	N-CA-C	-5.90	104.93	111.36
1	X	431	ILE	N-CA-C	-5.90	104.76	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	283	VAL	CB-CA-C	-5.90	104.08	112.22
1	X	267	GLU	CB-CA-C	5.86	120.17	110.90
1	X	364	ASN	CA-CB-CG	-5.84	106.76	112.60
1	X	320	ARG	CA-CB-CG	-5.76	102.58	114.10
1	X	422	LEU	N-CA-C	5.71	118.24	111.33
1	X	307	GLY	N-CA-C	5.58	119.43	112.73
1	X	280	ILE	CB-CA-C	-5.47	104.76	112.14
1	X	316	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	X	429	ARG	CB-CG-CD	5.37	123.66	111.30
1	X	272	PHE	N-CA-C	-5.25	105.61	112.23
1	X	447	PRO	N-CA-C	5.22	118.68	110.80
1	X	274	LYS	N-CA-C	-5.21	105.49	111.07
1	X	246	LEU	N-CA-C	-5.18	103.51	109.93
1	X	246	LEU	CB-CA-C	5.17	116.86	109.26
1	X	333	GLU	CA-C-O	-5.16	115.39	120.70
1	X	235	GLN	N-CA-C	5.13	118.67	111.74
1	X	397	ASP	CA-C-O	5.10	125.87	120.10
1	X	302	ILE	CB-CA-C	-5.08	105.21	112.22
1	X	444	VAL	N-CA-CB	5.06	116.36	110.65
1	X	459	PHE	N-CA-C	5.03	119.57	113.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	459	PHE	Peptide

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	X	1934	0	1893	66	2
2	X	6	0	0	4	0
3	X	24	0	4	9	0
4	X	10	0	0	1	0
All	All	1974	0	1897	66	2

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 18.

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:X:298:CYS:HB2	2:X:503:CAC:AS	2.03	1.19
1:X:416:HIS:O	1:X:420:LYS:HG3	1.68	0.92
1:X:298:CYS:HG	2:X:502:CAC:AS	1.61	0.91
1:X:313:MET:HE1	3:X:500:T44:I5'	2.49	0.83
1:X:277:THR:O	1:X:281:THR:HG23	1.81	0.78
1:X:250:ILE:O	1:X:340:GLN:NE2	2.16	0.77
1:X:331:ASN:C	1:X:333:GLU:H	1.92	0.77
1:X:451:PHE:HB3	1:X:456:LEU:HD21	1.68	0.75
1:X:439:PHE:HA	1:X:442:MET:HE3	1.68	0.75
1:X:264:VAL:HG11	1:X:446:CYS:SG	2.26	0.75
1:X:313:MET:CE	3:X:500:T44:I5'	3.12	0.67
1:X:331:ASN:O	1:X:333:GLU:N	2.27	0.67
1:X:435:HIS:CE1	3:X:500:T44:I5'	3.18	0.66
1:X:451:PHE:CB	1:X:456:LEU:HD21	2.25	0.66
1:X:276:ILE:O	1:X:280:ILE:HG12	1.96	0.65
1:X:337:THR:OG1	1:X:340:GLN:HG3	1.97	0.64
1:X:453:PRO:O	1:X:457:GLU:HG3	1.99	0.63
1:X:279:ALA:HB2	1:X:331:ASN:OD1	2.00	0.62
1:X:214:PRO:HB2	1:X:219:TRP:NE1	2.15	0.61
1:X:353:ILE:HD13	3:X:500:T44:I3	2.72	0.59
1:X:225:VAL:HG21	1:X:399:PHE:HE2	1.68	0.57
1:X:451:PHE:HB3	1:X:456:LEU:CD2	2.36	0.56
1:X:331:ASN:C	1:X:333:GLU:N	2.57	0.56
1:X:391:ARG:CZ	2:X:504:CAC:AS	3.14	0.55
1:X:233:ASN:O	1:X:234:ALA:C	2.50	0.53
1:X:310:MET:HE1	3:X:500:T44:I3	2.79	0.53
1:X:444:VAL:CG2	1:X:445:GLU:N	2.71	0.53
1:X:235:GLN:O	1:X:236:GLY:C	2.52	0.52
1:X:276:ILE:HG13	3:X:500:T44:I5	2.80	0.51
1:X:213:GLU:HB3	1:X:214:PRO:CD	2.41	0.51
1:X:276:ILE:HD11	3:X:500:T44:I5'	2.80	0.51
1:X:294:CYS:CB	2:X:501:CAC:AS	3.19	0.51
1:X:205:GLN:HE22	1:X:212:PRO:HB3	1.76	0.50
1:X:214:PRO:HB2	1:X:219:TRP:CD1	2.47	0.50
1:X:199:SER:O	1:X:201:MET:N	2.44	0.50
1:X:239:TRP:CD2	1:X:320:ARG:HD2	2.47	0.49
1:X:275:ILE:HD13	1:X:334:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:218:GLU:OE1	1:X:405:HIS:ND1	2.43	0.49
1:X:372:LEU:HD13	1:X:403:PHE:HA	1.95	0.49
1:X:250:ILE:HG12	1:X:267:GLU:OE2	2.13	0.48
1:X:277:THR:N	1:X:278:PRO:HD2	2.30	0.47
1:X:341:LEU:HD11	1:X:346:LEU:HD12	1.95	0.47
1:X:410:ARG:O	1:X:411:LYS:C	2.54	0.47
1:X:250:ILE:HA	1:X:267:GLU:OE2	2.14	0.47
1:X:415:THR:O	1:X:420:LYS:HE3	2.15	0.47
1:X:444:VAL:HG23	1:X:445:GLU:N	2.31	0.45
1:X:225:VAL:HG21	1:X:399:PHE:CE2	2.51	0.45
1:X:440:LEU:C	1:X:442:MET:H	2.25	0.44
1:X:328:LEU:CD1	1:X:354:PHE:CE1	3.01	0.44
1:X:250:ILE:HG23	1:X:267:GLU:HG2	1.99	0.44
1:X:370:VAL:O	1:X:374:GLN:HG3	2.16	0.44
1:X:451:PHE:N	1:X:451:PHE:CD1	2.86	0.43
1:X:328:LEU:HD12	1:X:354:PHE:CE1	2.54	0.43
1:X:363:PHE:O	1:X:364:ASN:C	2.59	0.43
1:X:342:LYS:HG3	1:X:347:GLY:HA2	2.01	0.41
1:X:435:HIS:NE2	3:X:500:T44:I5'	3.23	0.41
1:X:225:VAL:O	1:X:226:THR:C	2.62	0.41
1:X:225:VAL:HG12	1:X:371:ALA:HB1	2.02	0.41
1:X:268:ALA:O	1:X:269:PHE:C	2.64	0.41
1:X:429:ARG:HD3	4:X:5:HOH:O	2.19	0.41
1:X:205:GLN:NE2	1:X:212:PRO:HB3	2.35	0.41
1:X:277:THR:N	1:X:278:PRO:CD	2.84	0.41
1:X:308:CYS:O	1:X:309:CYS:C	2.61	0.41
1:X:246:LEU:HA	1:X:247:PRO:HD3	1.99	0.41
1:X:353:ILE:CD1	3:X:500:T44:I3	3.39	0.40
1:X:328:LEU:HG	1:X:354:PHE:CZ	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:201:MET:O	1:X:457:GLU:OE1[3_664]	1.28	0.92
1:X:201:MET:O	1:X:457:GLU:CD[3_664]	1.86	0.34

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	X	246/281 (88%)	229 (93%)	9 (4%)	8 (3%)	3	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	200	HIS
1	X	202	GLU
1	X	236	GLY
1	X	248	GLU
1	X	332	GLY
1	X	234	ALA
1	X	445	GLU
1	X	448	THR

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	X	206/246 (84%)	178 (86%)	28 (14%)	3	16

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	238	HIS
1	X	240	LYS
1	X	241	GLN

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Mol	Chain	Res	Type
1	X	242	LYS
1	X	243	ARG
1	X	248	GLU
1	X	267	GLU
1	X	270	SER
1	X	276	ILE
1	X	295	GLU
1	X	298	CYS
1	X	302	ILE
1	X	306	LYS
1	X	320	ARG
1	X	331	ASN
1	X	334	MET
1	X	359	SER
1	X	362	SER
1	X	373	LEU
1	X	381	SER
1	X	398	SER
1	X	411	LYS
1	X	415	THR
1	X	419	PRO
1	X	444	VAL
1	X	446	CYS
1	X	452	PRO
1	X	453	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	205	GLN
1	X	235	GLN
1	X	241	GLN
1	X	413	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are modelled with single atom - leaving 1 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	$\# Z > 2$
3	T44	X	500	-	24,25,25	1.53	5 (20%)	32,36,36	2.09	9 (28%)

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	T44	X	500	-	-	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	X	500	T44	C4'-C5'	3.07	1.46	1.40
3	X	500	T44	C3'-I3'	-2.96	2.03	2.10
3	X	500	T44	C4-C5	2.50	1.47	1.40
3	X	500	T44	O4-C4	-2.23	1.34	1.39
3	X	500	T44	C2'-C1'	-2.05	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	500	T44	O4'-C4'-C5'	6.06	135.95	120.30
3	X	500	T44	C4'-C5'-I5'	4.31	125.61	119.35
3	X	500	T44	O4'-C4'-C3'	-3.30	111.77	120.30
3	X	500	T44	C6'-C5'-I5'	-2.71	113.38	118.46
3	X	500	T44	C4'-C3'-I3'	-2.68	115.46	119.35
3	X	500	T44	C1-C7-CA	2.64	119.52	114.13
3	X	500	T44	O4-C1'-C6'	2.57	127.23	119.16
3	X	500	T44	C2'-C3'-C4'	2.08	125.25	121.33
3	X	500	T44	C6'-C1'-C2'	-2.04	117.89	120.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

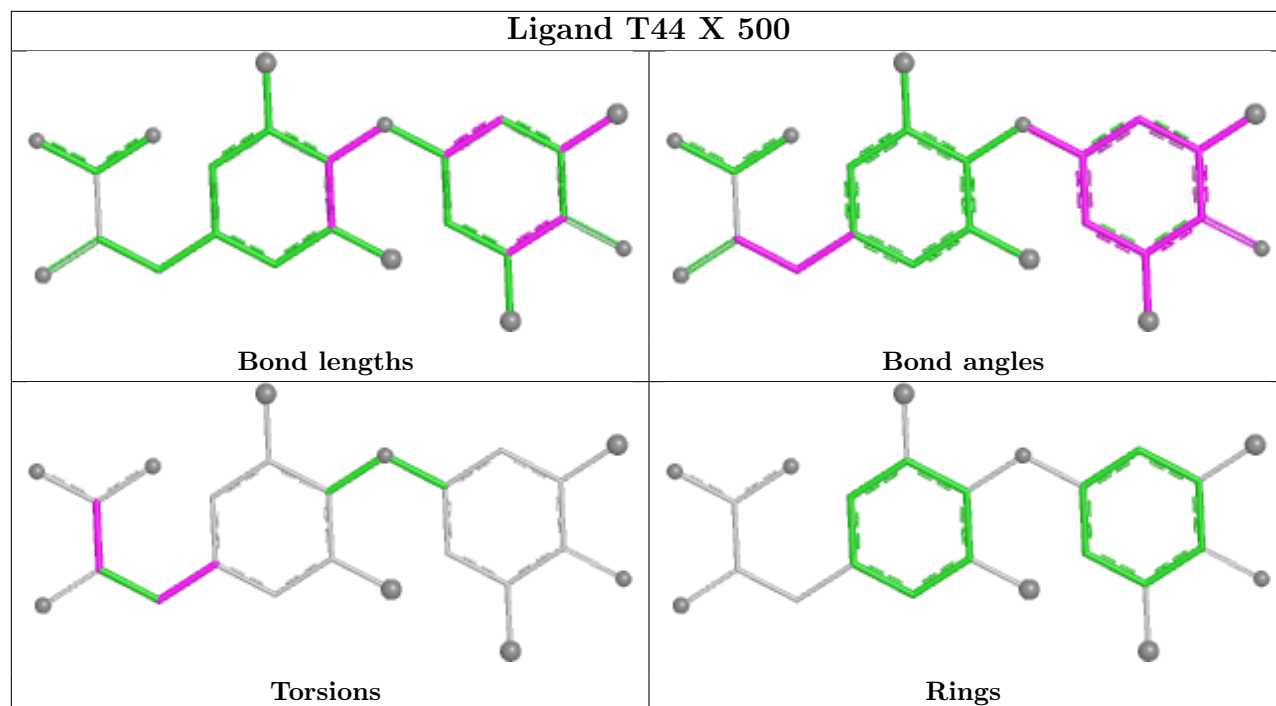
Mol	Chain	Res	Type	Atoms
3	X	500	T44	OXT-C-CA-C7
3	X	500	T44	O-C-CA-C7
3	X	500	T44	C6-C1-C7-CA

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	500	T44	9	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	X	250/281 (88%)	-0.18	7 (2%) 55 34	17, 52, 78, 99	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	282	ARG	6.4
1	X	240	LYS	6.4
1	X	460	GLU	3.3
1	X	251	GLY	3.2
1	X	264	VAL	2.3
1	X	200	HIS	2.2
1	X	199	SER	2.1

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 [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.

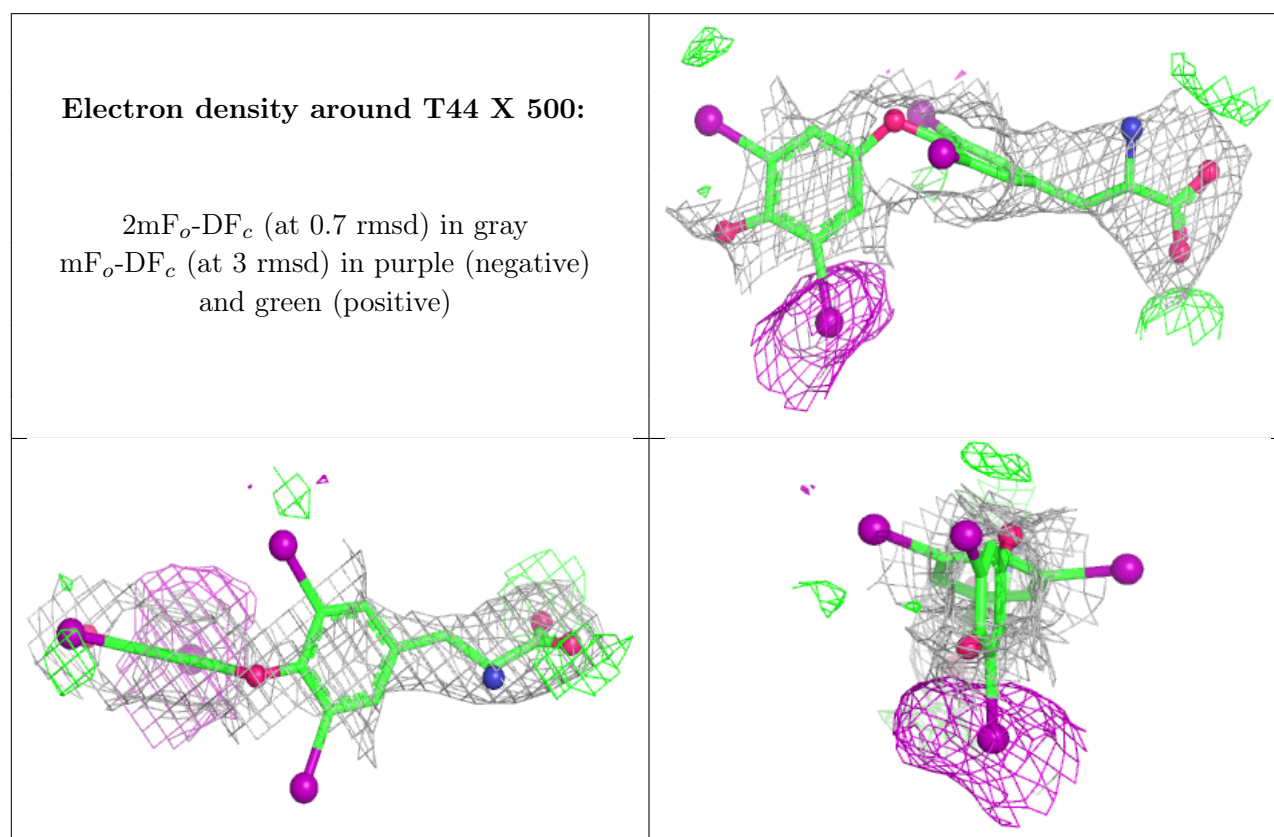
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CAC	X	503	1/5	-0.09	0.85	174,174,174,174	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CAC	X	502	1/5	0.71	0.18	97,97,97,97	1
2	CAC	X	501	1/5	0.88	0.16	82,82,82,82	1
2	CAC	X	505	1/5	0.90	0.18	51,51,51,51	1
2	CAC	X	504	1/5	0.92	0.14	65,65,65,65	1
2	CAC	X	506	1/5	0.94	0.28	61,61,61,61	1
3	T44	X	500	24/24	0.99	0.05	37,51,54,72	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.