Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 06:09 PM JST

PDB ID	:	9J0K / pdb_00009j0k
Title	:	An agonist(compound 14e)of Thyroid Hormone Receptor B
Authors	:	Yao, B.; Li, Y.
Deposited on	:	2024-08-02
Resolution	:	2.70 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:

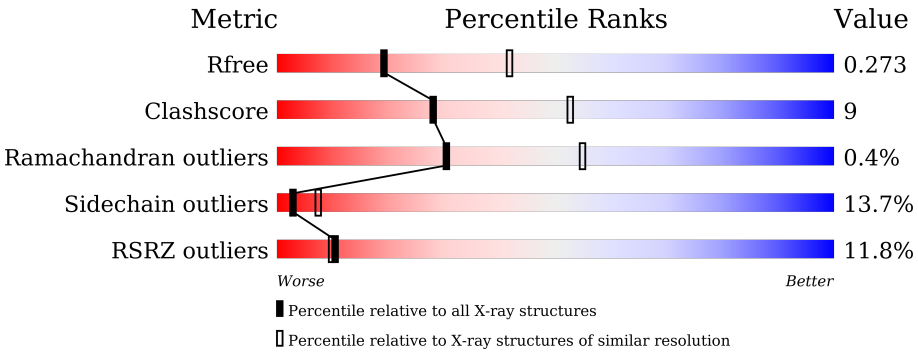
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	260	6% 67% 23% · 8%
1	B	260	17% 66% 24% · 6%
2	C	12	8% 42% 58%
2	D	12	8% 67% 25% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4128 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.

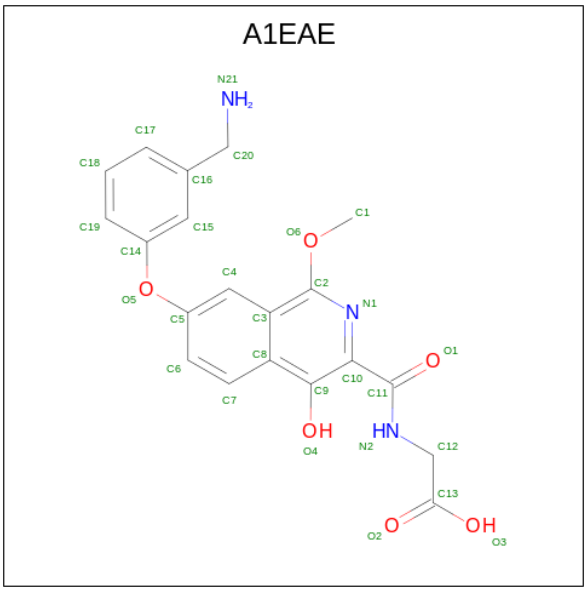
- Molecule 1 is a protein called Thyroid hormone receptor beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1900	1219	315	350	16			
1	B	244	Total	C	N	O	S	0	0	0
			1911	1228	318	349	16			

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	0	0	0
			102	65	17	20			
2	D	12	Total	C	N	O	0	0	0
			102	65	17	20			

- Molecule 3 is 2-[[7-[3-(aminomethyl)phenoxy]-1-methoxy-4-oxidanyl-isoquinolin-3-yl]carbonylamino]ethanoic acid (CCD ID: A1EAE) (formula: $C_{20}H_{19}N_3O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 29 20 3 6	0	0
3	B	1	Total C N O 29 20 3 6	0	0

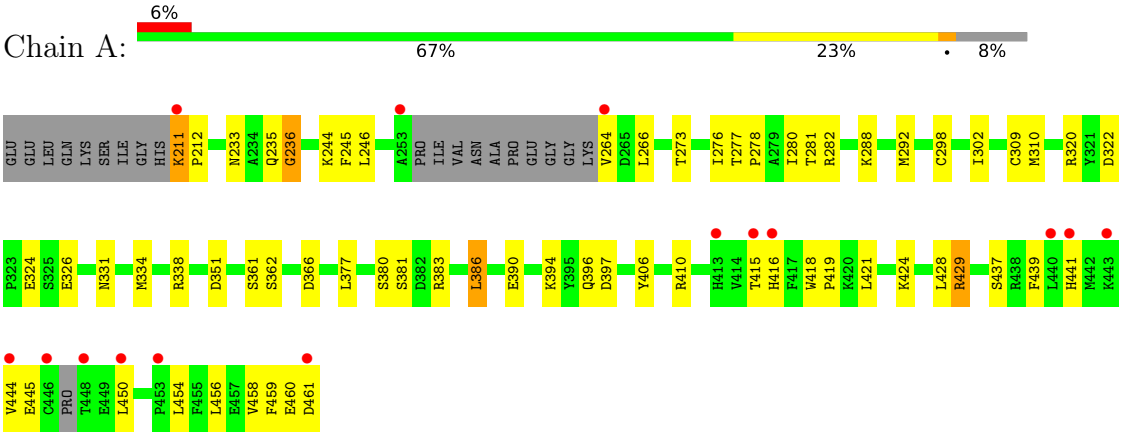
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	37	Total O 37 37	0	0
4	B	16	Total O 16 16	0	0
4	D	2	Total O 2 2	0	0

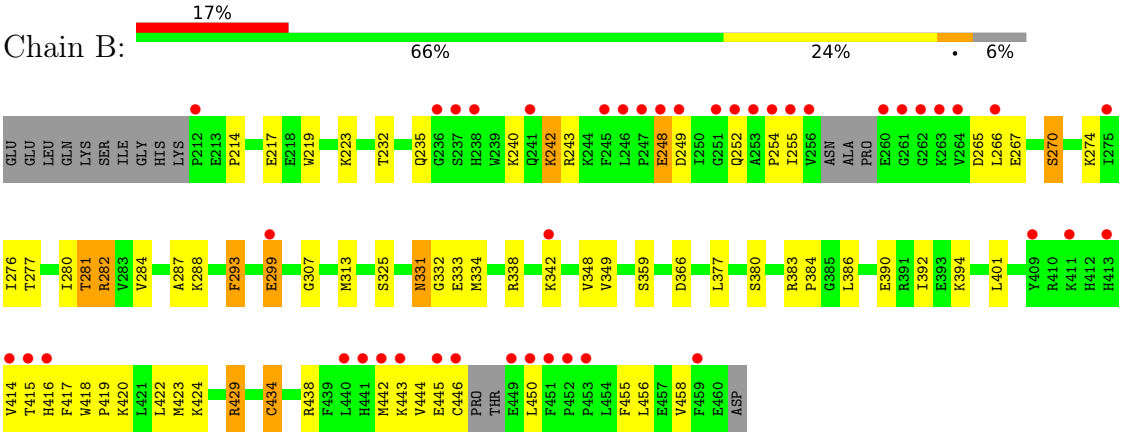
3 Residue-property plots (i)

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.

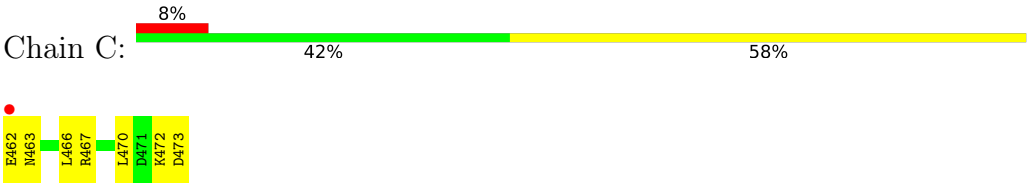
• Molecule 1: Thyroid hormone receptor beta



• Molecule 1: Thyroid hormone receptor beta

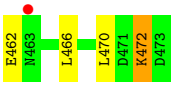


• Molecule 2: Nuclear receptor coactivator 2



• Molecule 2: Nuclear receptor coactivator 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	82.55Å 82.55Å 211.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.02 – 2.70 45.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.3 (45.02-2.70) 93.2 (45.02-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.224 , 0.275 0.225 , 0.273	Depositor DCC
R_{free} test set	1004 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4128	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EAE

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	1.19	3/1940 (0.2%)	1.42	5/2623 (0.2%)
1	B	1.06	0/1952	1.45	5/2641 (0.2%)
2	C	1.23	0/102	1.59	0/136
2	D	1.32	0/102	1.58	0/136
All	All	1.13	3/4096 (0.1%)	1.44	10/5536 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	ARG	C-O	5.46	1.30	1.23
1	A	245	PHE	C-O	-5.36	1.17	1.23
1	A	324	GLU	C-O	5.19	1.30	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	273	THR	CA-CB-OG1	-5.95	100.68	109.60
1	B	392	ILE	N-CA-C	-5.60	105.07	110.72
1	B	299	GLU	CB-CG-CD	5.39	121.77	112.60
1	B	417	PHE	N-CA-C	-5.39	104.27	112.04
1	A	397	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	293	PHE	CA-C-O	-5.32	115.24	120.82
1	B	331	ASN	CB-CA-C	-5.32	103.32	111.66
1	A	396	GLN	CA-C-O	-5.11	115.11	120.63
1	A	236	GLY	CA-C-N	5.06	128.00	120.31
1	A	236	GLY	C-N-CA	5.06	128.00	120.31

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	1900	0	1889	31	0
1	B	1911	0	1896	35	0
2	C	102	0	103	5	0
2	D	102	0	103	3	0
3	A	29	0	0	0	0
3	B	29	0	0	0	0
4	A	37	0	0	0	0
4	B	16	0	0	0	0
4	D	2	0	0	0	0
All	All	4128	0	3991	71	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 (71) 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:429:ARG:HH11	1:A:429:ARG:HG2	1.11	1.08
1:A:429:ARG:HG2	1:A:429:ARG:NH1	1.91	0.77
1:A:383:ARG:O	1:A:386:LEU:HD22	1.87	0.74
1:B:416:HIS:HD2	1:B:420:LYS:HD2	1.51	0.74
1:A:211:LYS:HB3	1:A:212:PRO:HD3	1.69	0.72
1:B:232:THR:O	1:B:282:ARG:HG2	1.90	0.71
1:B:419:PRO:O	1:B:423:MET:HG3	1.91	0.71
1:B:416:HIS:HD2	1:B:420:LYS:CD	2.04	0.70
1:A:338:ARG:HD3	1:A:351:ASP:OD1	1.92	0.69
1:A:418:TRP:HB3	1:A:419:PRO:HD3	1.76	0.67
2:C:463:ASN:O	2:C:467:ARG:HB2	1.96	0.66
1:B:445:GLU:O	1:B:446:CYS:HB2	1.95	0.66
1:A:383:ARG:HB2	1:A:386:LEU:HD13	1.77	0.65
1:B:307:GLY:HA3	1:B:383:ARG:NE	2.11	0.65
1:B:276:ILE:HG12	1:B:455:PHE:CD1	2.33	0.64
1:B:416:HIS:CD2	1:B:420:LYS:HD2	2.33	0.62
1:B:418:TRP:HB3	1:B:419:PRO:HD3	1.81	0.61
1:B:288:LYS:HD2	2:D:470:LEU:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:PHE:HZ	1:A:456:LEU:HD23	1.69	0.57
1:B:416:HIS:CD2	1:B:420:LYS:CD	2.87	0.55
1:A:421:LEU:O	1:A:424:LYS:HB2	2.08	0.54
1:B:383:ARG:HB2	1:B:386:LEU:HD11	1.90	0.53
1:B:307:GLY:HA3	1:B:383:ARG:HE	1.73	0.52
1:A:377:LEU:HD11	1:A:428:LEU:HD13	1.91	0.52
1:B:235:GLN:HG2	1:B:332:GLY:HA3	1.92	0.52
1:B:390:GLU:O	1:B:394:LYS:HG2	2.09	0.52
1:A:310:MET:HB2	1:A:459:PHE:CE1	2.45	0.52
1:A:439:PHE:CD1	1:A:439:PHE:O	2.63	0.52
1:B:276:ILE:HG12	1:B:455:PHE:HD1	1.76	0.51
1:A:322:ASP:O	1:A:326:GLU:N	2.43	0.51
1:B:349:VAL:HG22	1:B:434:CYS:HB3	1.93	0.50
1:A:310:MET:HB2	1:A:459:PHE:HE1	1.77	0.49
1:A:366:ASP:OD2	1:A:406:TYR:OH	2.24	0.49
1:B:248:GLU:O	1:B:252:GLN:HG2	2.13	0.49
1:A:278:PRO:O	1:A:282:ARG:HG3	2.13	0.48
1:A:380:SER:O	1:A:383:ARG:HG2	2.13	0.48
1:A:302:ILE:HD13	2:C:463:ASN:HB3	1.95	0.47
1:A:235:GLN:O	1:A:236:GLY:C	2.58	0.47
1:B:307:GLY:HA3	1:B:383:ARG:CD	2.45	0.47
1:B:270:SER:O	1:B:274:LYS:HG2	2.14	0.47
1:B:235:GLN:HG3	1:B:332:GLY:O	2.15	0.46
1:A:441:HIS:HA	1:A:444:VAL:HG22	1.99	0.45
2:C:463:ASN:HB2	2:C:467:ARG:NH1	2.32	0.45
1:A:338:ARG:NH1	1:A:351:ASP:HA	2.31	0.45
1:B:415:THR:O	1:B:416:HIS:C	2.59	0.45
1:A:277:THR:HB	1:A:278:PRO:CD	2.46	0.44
1:A:277:THR:HB	1:A:278:PRO:HD3	1.99	0.44
1:B:359:SER:OG	1:B:424:LYS:HE3	2.18	0.44
1:B:307:GLY:HA3	1:B:383:ARG:HD2	1.99	0.44
1:A:276:ILE:O	1:A:280:ILE:HG13	2.16	0.44
1:B:214:PRO:HB2	1:B:219:TRP:CD1	2.53	0.43
2:C:466:LEU:HD23	2:C:466:LEU:HA	1.85	0.43
1:A:280:ILE:HG21	1:A:458:VAL:HG21	2.01	0.43
1:B:280:ILE:HG21	1:B:458:VAL:HG21	2.01	0.43
1:B:287:ALA:O	1:B:293:PHE:CD2	2.72	0.43
1:A:454:LEU:HD12	1:A:454:LEU:HA	1.83	0.42
2:D:466:LEU:HA	2:D:466:LEU:HD23	1.67	0.42
1:B:438:ARG:O	1:B:442:MET:N	2.50	0.42
1:B:429:ARG:HE	1:B:429:ARG:HB3	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:472:LYS:HB3	2:D:472:LYS:HE3	1.90	0.42
1:A:450:LEU:HA	1:A:450:LEU:HD23	1.80	0.41
1:B:281:THR:O	1:B:284:VAL:HG22	2.20	0.41
1:A:421:LEU:HD12	1:A:421:LEU:HA	1.91	0.41
1:A:288:LYS:HD2	2:C:470:LEU:HA	2.03	0.41
1:B:331:ASN:HD22	1:B:331:ASN:N	2.19	0.41
1:B:383:ARG:HA	1:B:384:PRO:HD3	1.92	0.41
1:A:280:ILE:HG23	1:A:309:CYS:SG	2.61	0.41
1:A:246:LEU:HD22	1:A:334:MET:HE3	2.02	0.40
1:B:242:LYS:HA	1:B:242:LYS:HD2	1.87	0.40
1:B:377:LEU:O	1:B:380:SER:OG	2.29	0.40
1:B:416:HIS:CD2	1:B:420:LYS:HD3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	234/260 (90%)	222 (95%)	12 (5%)	0	100 100
1	B	238/260 (92%)	220 (92%)	16 (7%)	2 (1%)	16 38
2	C	10/12 (83%)	8 (80%)	2 (20%)	0	100 100
2	D	10/12 (83%)	10 (100%)	0	0	100 100
All	All	492/544 (90%)	460 (94%)	30 (6%)	2 (0%)	30 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	ASP
1	B	254	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	209/228 (92%)	186 (89%)	23 (11%)	5 12
1	B	207/228 (91%)	175 (84%)	32 (16%)	2 6
2	C	11/11 (100%)	8 (73%)	3 (27%)	0 1
2	D	11/11 (100%)	9 (82%)	2 (18%)	1 4
All	All	438/478 (92%)	378 (86%)	60 (14%)	3 7

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LYS
1	A	233	ASN
1	A	244	LYS
1	A	264	VAL
1	A	266	LEU
1	A	281	THR
1	A	292	MET
1	A	298	CYS
1	A	331	ASN
1	A	361	SER
1	A	362	SER
1	A	381	SER
1	A	386	LEU
1	A	390	GLU
1	A	394	LYS
1	A	410	ARG
1	A	415	THR
1	A	416	HIS
1	A	429	ARG
1	A	437	SER
1	A	445	GLU
1	A	460	GLU
1	A	461	ASP
1	B	217	GLU

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Mol	Chain	Res	Type
1	B	223	LYS
1	B	240	LYS
1	B	242	LYS
1	B	243	ARG
1	B	248	GLU
1	B	249	ASP
1	B	255	ILE
1	B	266	LEU
1	B	267	GLU
1	B	270	SER
1	B	277	THR
1	B	281	THR
1	B	282	ARG
1	B	299	GLU
1	B	313	MET
1	B	325	SER
1	B	333	GLU
1	B	334	MET
1	B	338	ARG
1	B	342	LYS
1	B	348	VAL
1	B	366	ASP
1	B	401	LEU
1	B	414	VAL
1	B	422	LEU
1	B	429	ARG
1	B	434	CYS
1	B	443	LYS
1	B	444	VAL
1	B	450	LEU
1	B	456	LEU
2	C	462	GLU
2	C	472	LYS
2	C	473	ASP
2	D	462	GLU
2	D	472	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	252	GLN

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Mol	Chain	Res	Type
1	A	331	ASN
1	B	233	ASN
1	B	241	GLN
1	B	331	ASN
1	B	340	GLN
1	B	412	HIS
1	B	416	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides 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	A1EAE	B	501	-	30,31,31	0.78	1 (3%)	39,43,43	1.73	11 (28%)
3	A1EAE	A	501	-	30,31,31	0.80	0	39,43,43	1.23	4 (10%)

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	A1EAE	B	501	-	-	6/17/17/17	0/3/3/3
3	A1EAE	A	501	-	-	1/17/17/17	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	A1EAE	C9-C10	2.08	1.43	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	A1EAE	C10-C11-N2	5.40	120.94	115.67
3	B	501	A1EAE	O5-C5-C6	3.14	130.44	119.38
3	B	501	A1EAE	C14-O5-C5	3.00	125.81	118.80
3	B	501	A1EAE	C7-C8-C9	2.82	125.16	121.42
3	A	501	A1EAE	C3-C2-N1	-2.79	122.46	124.40
3	B	501	A1EAE	C11-C10-N1	-2.75	113.42	115.99
3	B	501	A1EAE	C10-N1-C2	2.70	121.70	114.62
3	B	501	A1EAE	O5-C5-C4	-2.66	108.95	119.84
3	A	501	A1EAE	C11-C10-N1	2.58	118.40	115.99
3	B	501	A1EAE	O4-C9-C8	2.43	121.79	116.64
3	B	501	A1EAE	C3-C2-N1	-2.37	122.75	124.40
3	A	501	A1EAE	C2-C3-C8	2.32	118.77	115.93
3	A	501	A1EAE	C9-C8-C3	-2.30	117.36	119.45
3	B	501	A1EAE	C9-C8-C3	-2.23	117.42	119.45
3	B	501	A1EAE	C2-C3-C8	2.10	118.51	115.93

There are no chirality outliers.

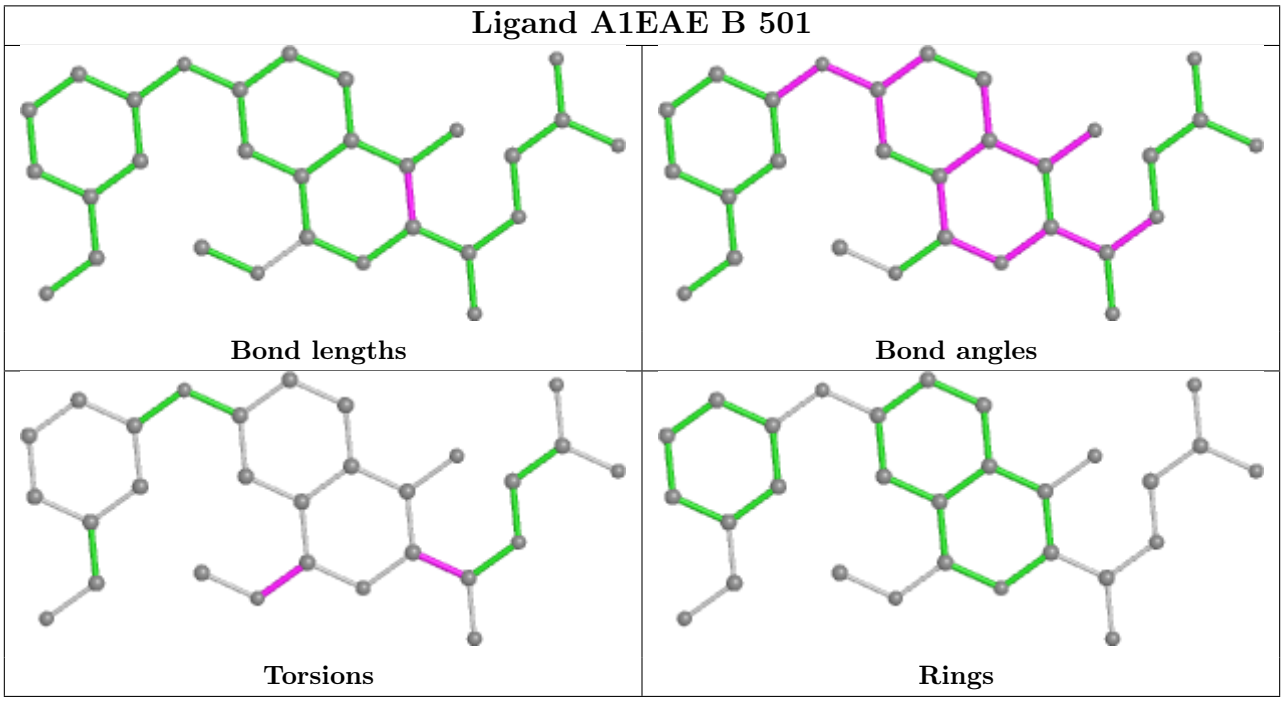
All (7) torsion outliers are listed below:

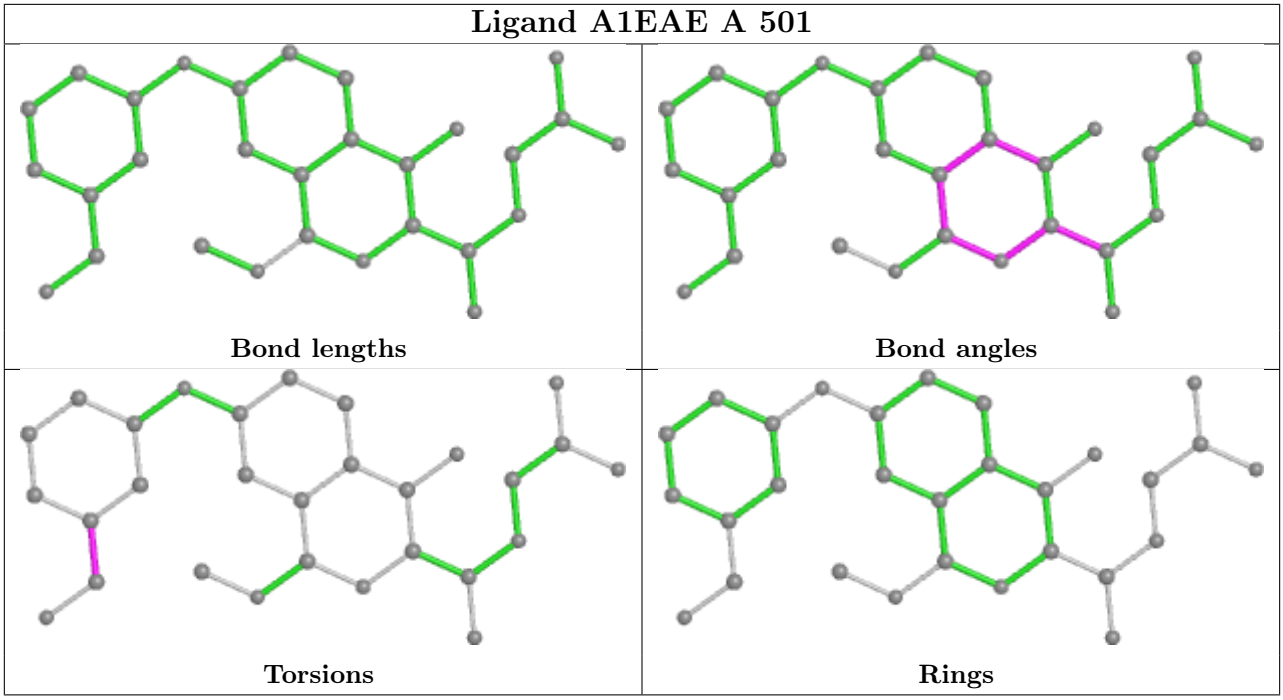
Mol	Chain	Res	Type	Atoms
3	B	501	A1EAE	C9-C10-C11-O1
3	B	501	A1EAE	C9-C10-C11-N2
3	B	501	A1EAE	N1-C10-C11-O1
3	B	501	A1EAE	N1-C10-C11-N2
3	B	501	A1EAE	N1-C2-O6-C1
3	B	501	A1EAE	C3-C2-O6-C1
3	A	501	A1EAE	C15-C16-C20-N21

There are no ring outliers.

No monomer is involved in short contacts.

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.





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	240/260 (92%)	0.32	15 (6%) 27 25	17, 45, 100, 131	0
1	B	244/260 (93%)	1.03	43 (17%) 4 5	28, 69, 126, 150	0
2	C	12/12 (100%)	0.33	1 (8%) 19 17	32, 53, 79, 95	0
2	D	12/12 (100%)	0.88	1 (8%) 19 17	44, 54, 79, 90	0
All	All	508/544 (93%)	0.68	60 (11%) 10 10	17, 57, 117, 150	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	CYS	7.1
1	B	256	VAL	7.0
1	B	416	HIS	5.4
1	B	255	ILE	5.2
1	B	449	GLU	5.2
1	B	212	PRO	5.1
1	B	445	GLU	4.9
1	B	414	VAL	4.9
1	B	413	HIS	4.8
1	A	264	VAL	4.7
1	B	450	LEU	4.5
1	A	253	ALA	4.3
1	A	450	LEU	4.3
1	B	251	GLY	4.1
1	B	446	CYS	3.9
1	B	260	GLU	3.5
1	A	416	HIS	3.5
1	B	253	ALA	3.4
1	A	415	THR	3.4
1	A	211	LYS	3.4
1	A	440	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	415	THR	3.2
1	B	245	PHE	3.1
1	B	440	LEU	3.1
1	B	252	GLN	3.1
1	B	299	GLU	3.0
1	A	448	THR	3.0
1	B	254	PRO	3.0
1	B	248	GLU	2.8
1	B	342	LYS	2.8
1	B	263	LYS	2.7
1	B	409	TYR	2.7
1	A	444	VAL	2.7
1	B	451	PHE	2.7
1	B	237	SER	2.7
1	A	443	LYS	2.6
1	B	264	VAL	2.6
1	A	453	PRO	2.6
1	B	453	PRO	2.5
1	B	249	ASP	2.5
1	B	266	LEU	2.5
1	B	236	GLY	2.4
1	A	461	ASP	2.4
2	D	463	ASN	2.4
1	B	246	LEU	2.4
1	B	411	LYS	2.4
1	B	443	LYS	2.4
1	B	238	HIS	2.3
1	B	241	GLN	2.3
2	C	462	GLU	2.2
1	B	459	PHE	2.2
1	B	262	GLY	2.2
1	B	261	GLY	2.2
1	A	413	HIS	2.1
1	A	441	HIS	2.1
1	B	441	HIS	2.1
1	B	442	MET	2.1
1	B	452	PRO	2.1
1	B	247	PRO	2.0
1	B	275	ILE	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 (i)

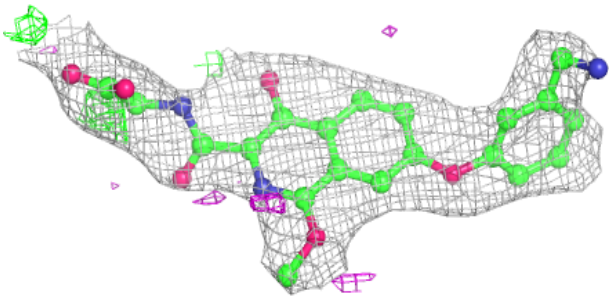
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

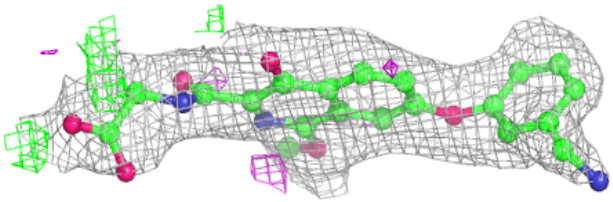
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A1EAE	B	501	29/29	0.88	0.15	44,52,66,72	0
3	A1EAE	A	501	29/29	0.96	0.08	26,29,48,50	0

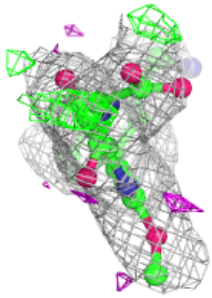
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1EAE 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)

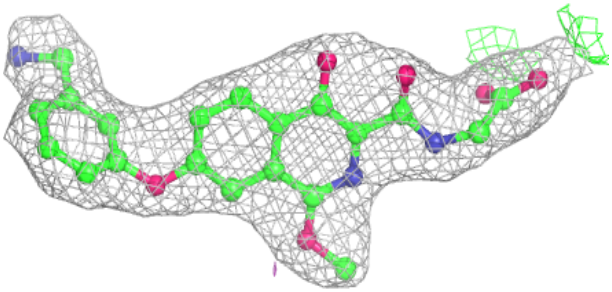


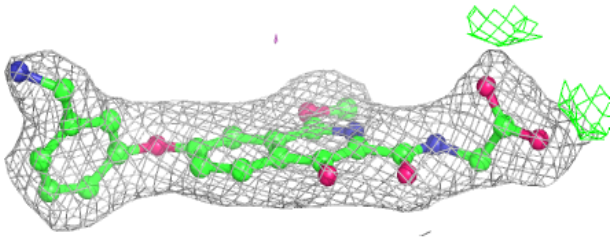


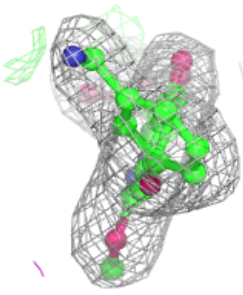


Electron density around A1EAE A 501:

$2mF_o$-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.