



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:06 AM UTC

PDB ID : 1N46 / pdb_00001n46
Title : CRYSTAL STRUCTURE OF HUMAN TR BETA LIGAND-BINDING DOMAIN COMPLEXED WITH A POTENT SUBTYPE-SELECTIVE THYROMIMETIC
Authors : Dow, R.L.; Schneider, S.R.; Paight, E.S.; Hank, R.F.; Chiang, P.; Cornelius, P.; Lee, E.; Newsome, W.P.; Swick, A.G.; Spitzer, J.; Hargrove, D.M.; Patterson, T.A.; Pandit, J.; Chrunyk, B.A.; LeMotte, P.K.; Danley, D.E.; Rosner, M.H.; Ammirati, M.J.; Simons, S.P.; Schulte, G.K.; Tate, B.F.; DaSilva-Jardine, P.
Deposited on : 2002-10-30
Resolution : 2.20 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

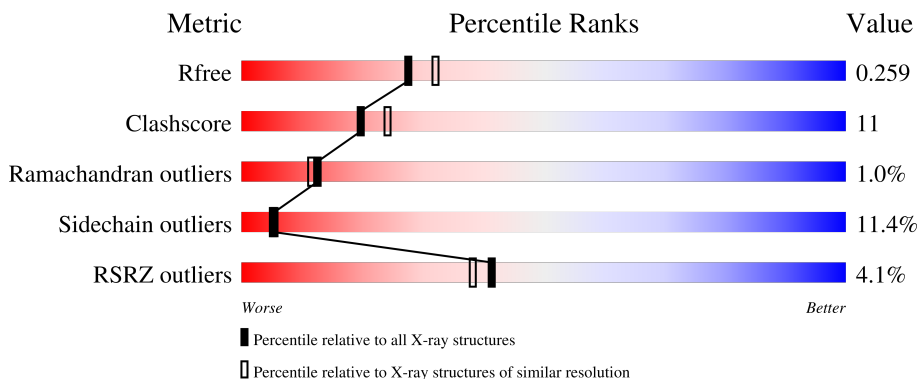
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	258	
1	B	258	

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

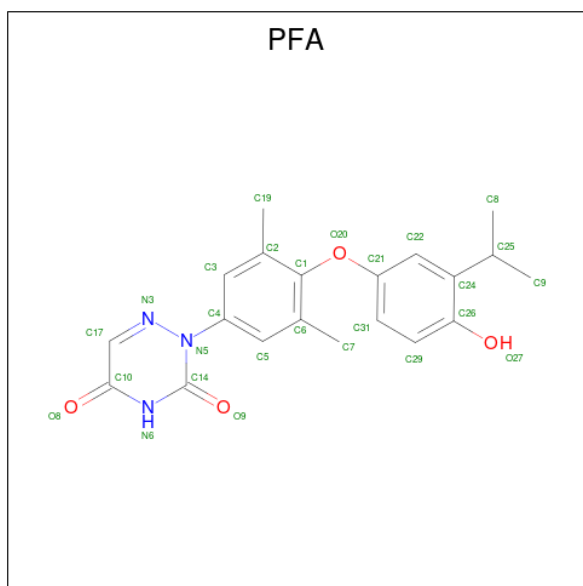
There are 3 unique types of molecules in this entry. The entry contains 4040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	A	248	Total	C	N	O	S	0	0	0
			1968	1264	326	362	16			
1	B	239	Total	C	N	O	S	0	0	0
			1904	1223	315	350	16			

- Molecule 2 is [4-(4-HYDROXY-3-ISOPROPYL-PHENOXY)-3,5-DIMETHYL-PHENYL]-6-AZAURACIL (CCD ID: PFA) (formula: C₂₀H₂₁N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	20	3	4		
2	B	1	Total	C	N	O	0	0
			27	20	3	4		

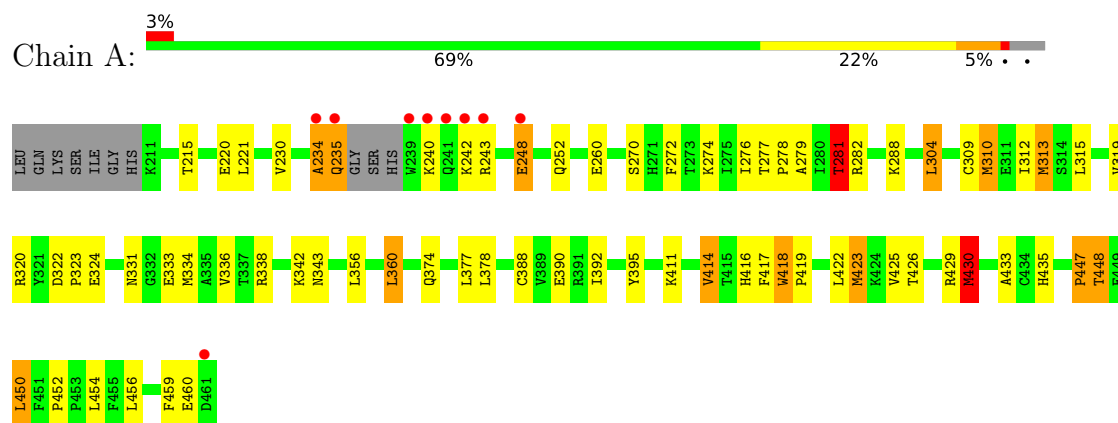
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total 85	O 85	0	0
3	B	29	Total 29	O 29	0	0

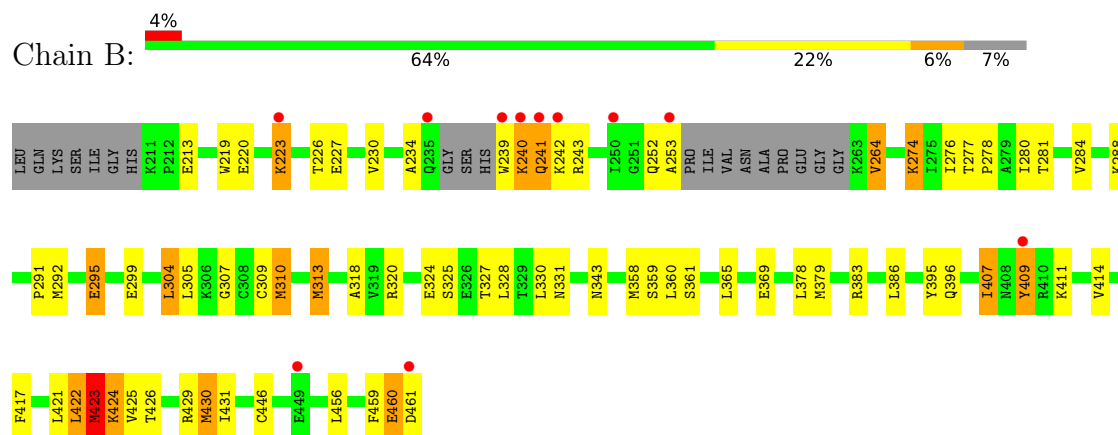
3 Residue-property plots [i](#)

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-1



• Molecule 1: Thyroid hormone receptor Beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.92Å 105.31Å 55.99Å 90.00° 98.19° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-2.20) 96.6 (30.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.192 , 0.256 0.197 , 0.259	Depositor DCC
R_{free} test set	1226 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4040	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.93% 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: PFA

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	1.48	10/2012 (0.5%)	1.40	8/2722 (0.3%)
1	B	1.36	6/1945 (0.3%)	1.38	8/2628 (0.3%)
All	All	1.42	16/3957 (0.4%)	1.39	16/5350 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	313	MET	SD-CE	-15.79	1.40	1.79
1	A	313	MET	SD-CE	-15.77	1.40	1.79
1	A	423	MET	SD-CE	-11.35	1.51	1.79
1	A	452	PRO	CA-C	8.96	1.56	1.51
1	A	430	MET	SD-CE	-8.72	1.57	1.79
1	B	310	MET	SD-CE	-7.88	1.59	1.79
1	B	423	MET	SD-CE	-7.14	1.61	1.79
1	A	418	TRP	C-O	-6.97	1.18	1.24
1	A	310	MET	SD-CE	-6.21	1.64	1.79
1	A	430	MET	C-O	-6.16	1.16	1.24
1	A	334	MET	SD-CE	5.84	1.94	1.79
1	B	431	ILE	CA-C	-5.55	1.46	1.52
1	A	281	THR	CA-CB	5.51	1.62	1.53
1	A	395	TYR	C-O	-5.20	1.18	1.24
1	B	430	MET	CG-SD	-5.14	1.68	1.80
1	B	318	ALA	CA-CB	-5.05	1.45	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	MET	CB-CA-C	-6.87	99.18	110.85
1	A	338	ARG	CA-CB-CG	6.80	127.71	114.10
1	A	430	MET	N-CA-CB	6.32	119.51	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	383	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	A	448	THR	N-CA-CB	-5.60	101.03	110.49
1	B	274	LYS	N-CA-C	-5.59	105.27	111.36
1	A	338	ARG	NE-CZ-NH2	-5.56	114.20	119.20
1	B	242	LYS	N-CA-C	-5.52	105.48	113.21
1	B	430	MET	CA-CB-CG	-5.45	103.20	114.10
1	B	307	GLY	N-CA-C	-5.42	105.83	112.77
1	A	315	LEU	N-CA-C	-5.27	105.23	110.97
1	B	241	GLN	CA-C-N	5.14	127.99	119.35
1	B	241	GLN	C-N-CA	5.14	127.99	119.35
1	A	447	PRO	CA-C-O	5.11	126.86	121.03
1	B	328	LEU	N-CA-C	-5.05	102.05	110.17
1	A	215	THR	N-CA-C	-5.03	104.22	110.41

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	1968	0	1972	48	0
1	B	1904	0	1902	50	0
2	A	27	0	21	5	0
2	B	27	0	21	6	0
3	A	85	0	0	3	0
3	B	29	0	0	2	0
All	All	4040	0	3916	90	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 11.

All (90) 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:310:MET:HE1	2:A:462:PFA:H29C	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:MET:HA	1:A:313:MET:HE3	1.61	0.83
1:B:429:ARG:HB3	3:B:13:HOH:O	1.78	0.82
1:B:291:PRO:O	1:B:295:GLU:HG2	1.86	0.76
1:A:423:MET:HE2	1:B:227:GLU:HG2	1.67	0.76
1:A:390:GLU:HG2	3:A:90:HOH:O	1.87	0.75
1:B:310:MET:HA	1:B:313:MET:HE3	1.68	0.75
1:A:310:MET:CE	2:A:462:PFA:H29C	2.19	0.71
1:B:320:ARG:HH22	2:B:463:PFA:HN6	1.39	0.71
1:B:310:MET:HE2	1:B:313:MET:HE3	1.72	0.70
1:B:309:CYS:SG	1:B:313:MET:HE2	2.32	0.69
1:A:320:ARG:HH22	2:A:462:PFA:HN6	1.44	0.65
1:A:456:LEU:O	1:A:460:GLU:HB2	1.96	0.65
1:A:423:MET:HE1	1:B:230:VAL:CG2	2.27	0.64
1:B:423:MET:HA	1:B:423:MET:HE3	1.80	0.63
1:A:430:MET:HE3	1:B:223:LYS:HA	1.82	0.61
1:A:310:MET:HE1	2:A:462:PFA:C29	2.30	0.61
1:B:310:MET:HE2	1:B:313:MET:CE	2.30	0.61
1:A:423:MET:HE1	1:B:230:VAL:HG23	1.83	0.60
1:B:253:ALA:HB2	1:B:343:ASN:HD21	1.65	0.60
1:B:456:LEU:O	1:B:460:GLU:HB3	2.00	0.60
1:A:310:MET:HE3	1:A:435:HIS:CE1	2.37	0.60
1:A:281:THR:HG22	1:A:454:LEU:CD2	2.32	0.59
1:A:430:MET:CE	1:B:223:LYS:HA	2.33	0.59
1:B:310:MET:CE	2:B:463:PFA:H29C	2.33	0.58
1:A:277:THR:O	1:A:281:THR:HG23	2.04	0.58
1:B:313:MET:HE1	1:B:459:PHE:HZ	1.68	0.57
1:B:213:GLU:CD	1:B:409:TYR:HB2	2.29	0.57
1:A:433:ALA:HB1	1:B:409:TYR:OH	2.05	0.57
1:B:310:MET:HE1	2:B:463:PFA:H29C	1.86	0.57
1:B:304:LEU:HD13	1:B:386:LEU:HD21	1.88	0.56
1:A:429:ARG:HB3	3:A:45:HOH:O	2.06	0.56
1:A:248:GLU:HA	1:A:248:GLU:OE1	2.07	0.54
1:A:248:GLU:OE1	1:A:252:GLN:OE1	2.24	0.54
1:B:264:VAL:HG11	1:B:446:CYS:SG	2.48	0.54
1:B:325:SER:HB2	1:B:327:THR:HG23	1.88	0.54
1:A:310:MET:HE2	1:A:313:MET:CE	2.39	0.53
1:A:260:GLU:HG2	1:A:343:ASN:HD21	1.74	0.53
1:B:414:VAL:HG22	1:B:417:PHE:HD1	1.75	0.52
1:A:234:ALA:C	1:A:235:GLN:HG2	2.34	0.52
1:A:309:CYS:SG	1:A:313:MET:HE2	2.49	0.52
1:A:418:TRP:HB3	1:A:419:PRO:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLU:OE2	1:B:409:TYR:HB2	2.11	0.51
1:B:313:MET:O	2:B:463:PFA:HC3	2.10	0.50
1:B:407:ILE:CG1	1:B:417:PHE:HE2	2.24	0.50
1:B:421:LEU:O	1:B:424:LYS:HB2	2.11	0.50
1:B:310:MET:HA	1:B:310:MET:HE2	1.94	0.50
1:A:281:THR:HG22	1:A:454:LEU:HD21	1.92	0.49
1:B:239:TRP:O	1:B:240:LYS:C	2.55	0.49
1:A:426:THR:HG23	3:A:95:HOH:O	2.12	0.49
1:A:272:PHE:HE1	1:A:336:VAL:HG11	1.78	0.49
1:B:219:TRP:O	1:B:223:LYS:HD3	2.12	0.48
1:A:414:VAL:HG22	1:A:417:PHE:HD1	1.78	0.48
1:B:280:ILE:O	1:B:284:VAL:HG23	2.14	0.48
1:B:379:MET:O	1:B:396:GLN:HB2	2.13	0.47
1:A:447:PRO:HG2	1:A:450:LEU:HD11	1.96	0.47
1:A:356:LEU:HG	1:A:360:LEU:HD22	1.97	0.47
1:B:277:THR:HB	1:B:278:PRO:HD3	1.97	0.46
1:A:272:PHE:HB3	2:A:462:PFA:HC93	1.98	0.46
1:B:407:ILE:HG12	1:B:417:PHE:HE2	1.81	0.46
1:A:270:SER:HB3	1:A:450:LEU:HD22	1.98	0.46
1:B:429:ARG:HD2	3:B:8:HOH:O	2.15	0.46
1:A:310:MET:HE2	1:A:313:MET:HE3	1.98	0.46
1:B:365:LEU:HA	1:B:369:GLU:OE1	2.15	0.45
1:B:292:MET:HG2	1:B:395:TYR:CE1	2.52	0.45
1:B:409:TYR:CD2	1:B:409:TYR:C	2.94	0.45
1:A:422:LEU:HD23	1:A:422:LEU:HA	1.78	0.44
1:A:279:ALA:HB2	1:A:331:ASN:HD21	1.83	0.44
1:A:304:LEU:HG	1:A:378:LEU:O	2.18	0.44
1:B:276:ILE:HD12	2:B:463:PFA:HC71	2.00	0.44
1:A:377:LEU:HD23	1:A:425:VAL:HG13	1.99	0.44
1:A:423:MET:CE	1:B:227:GLU:HG2	2.45	0.44
1:B:226:THR:O	1:B:230:VAL:HG22	2.18	0.44
1:B:304:LEU:HG	1:B:378:LEU:O	2.18	0.44
1:B:409:TYR:O	1:B:409:TYR:CG	2.70	0.43
1:B:264:VAL:HG12	1:B:264:VAL:O	2.18	0.43
1:B:304:LEU:HD12	1:B:304:LEU:HA	1.81	0.43
1:A:388:CYS:O	1:A:392:ILE:HD12	2.19	0.42
1:A:416:HIS:HB3	1:A:419:PRO:HG2	2.01	0.42
1:A:313:MET:HE1	1:A:459:PHE:HZ	1.85	0.42
1:A:277:THR:N	1:A:278:PRO:HD2	2.34	0.42
1:A:312:ILE:HG23	1:A:374:GLN:HG2	2.01	0.42
1:A:430:MET:HE3	1:B:223:LYS:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:MET:HE2	1:A:313:MET:HE1	2.02	0.42
1:A:278:PRO:O	1:A:282:ARG:HG3	2.20	0.41
1:A:322:ASP:HA	1:A:323:PRO:HD3	1.84	0.41
1:A:418:TRP:HB3	1:A:419:PRO:HD3	2.02	0.41
1:B:310:MET:HE1	2:B:463:PFA:C29	2.50	0.41
1:B:330:LEU:O	1:B:331:ASN:HB2	2.21	0.40
1:B:422:LEU:O	1:B:425:VAL:HB	2.22	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	244/258 (95%)	236 (97%)	7 (3%)	1 (0%)	30	34
1	B	233/258 (90%)	222 (95%)	7 (3%)	4 (2%)	7	5
All	All	477/516 (92%)	458 (96%)	14 (3%)	5 (1%)	12	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	ALA
1	A	234	ALA
1	B	411	LYS
1	B	240	LYS
1	B	264	VAL

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	218/226 (96%)	195 (89%)	23 (11%)	6	6
1	B	211/226 (93%)	185 (88%)	26 (12%)	4	4
All	All	429/452 (95%)	380 (89%)	49 (11%)	5	5

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	GLU
1	A	221	LEU
1	A	230	VAL
1	A	235	GLN
1	A	240	LYS
1	A	242	LYS
1	A	243	ARG
1	A	248	GLU
1	A	274	LYS
1	A	276	ILE
1	A	281	THR
1	A	288	LYS
1	A	304	LEU
1	A	319	VAL
1	A	324	GLU
1	A	333	GLU
1	A	342	LYS
1	A	360	LEU
1	A	411	LYS
1	A	414	VAL
1	A	430	MET
1	A	448	THR
1	A	450	LEU
1	B	220	GLU
1	B	223	LYS
1	B	241	GLN
1	B	243	ARG
1	B	252	GLN
1	B	274	LYS
1	B	281	THR
1	B	288	LYS
1	B	295	GLU
1	B	299	GLU

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Mol	Chain	Res	Type
1	B	304	LEU
1	B	305	LEU
1	B	324	GLU
1	B	358	MET
1	B	359	SER
1	B	360	LEU
1	B	361	SER
1	B	407	ILE
1	B	409	TYR
1	B	422	LEU
1	B	423	MET
1	B	424	LYS
1	B	426	THR
1	B	430	MET
1	B	460	GLU
1	B	461	ASP

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

Mol	Chain	Res	Type
1	A	252	GLN
1	A	331	ASN
1	B	252	GLN
1	B	343	ASN

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
2	PFA	B	463	-	27,29,29	1.93	10 (37%)	37,42,42	2.15	8 (21%)
2	PFA	A	462	-	27,29,29	1.72	5 (18%)	37,42,42	2.44	15 (40%)

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
2	PFA	B	463	-	-	2/12/12/12	0/3/3/3
2	PFA	A	462	-	-	1/12/12/12	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	463	PFA	C17-N3	-3.67	1.25	1.29
2	B	463	PFA	C3-C2	3.63	1.44	1.39
2	B	463	PFA	C31-C21	3.61	1.45	1.38
2	A	462	PFA	C5-C4	3.54	1.45	1.39
2	A	462	PFA	C22-C21	3.41	1.44	1.39
2	A	462	PFA	C31-C21	3.30	1.44	1.38
2	B	463	PFA	C1-C2	3.02	1.45	1.40
2	B	463	PFA	C3-C4	2.76	1.44	1.39
2	B	463	PFA	C10-N6	-2.50	1.34	1.38
2	A	462	PFA	C7-C6	-2.40	1.46	1.51
2	B	463	PFA	C1-C6	2.37	1.44	1.40
2	B	463	PFA	C24-C25	2.27	1.55	1.52
2	B	463	PFA	C4-N5	-2.22	1.39	1.43
2	A	462	PFA	C5-C6	2.14	1.42	1.39
2	B	463	PFA	C22-C21	2.11	1.42	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	463	PFA	O8-C10-C17	-6.17	116.31	123.77
2	A	462	PFA	C4-N5-C14	5.77	127.62	120.83
2	A	462	PFA	C3-C4-N5	5.49	127.22	119.27
2	B	463	PFA	C10-N6-C14	-4.79	120.67	126.61
2	A	462	PFA	O8-C10-C17	-4.75	118.02	123.77
2	B	463	PFA	C5-C4-N5	-4.74	112.40	119.27
2	A	462	PFA	C5-C4-N5	-4.34	112.97	119.27
2	B	463	PFA	C3-C4-N5	4.27	125.45	119.27
2	A	462	PFA	C10-N6-C14	-3.96	121.70	126.61
2	B	463	PFA	O8-C10-N6	3.54	124.41	119.27
2	B	463	PFA	C4-C5-C6	-3.39	118.18	121.55
2	A	462	PFA	C4-C5-C6	-3.30	118.27	121.55
2	A	462	PFA	C9-C25-C24	-3.27	106.06	111.71
2	A	462	PFA	O8-C10-N6	3.25	123.99	119.27
2	B	463	PFA	C9-C25-C8	-3.15	103.74	110.23
2	A	462	PFA	C29-C31-C21	-2.88	116.44	119.73
2	A	462	PFA	C17-N3-N5	2.82	121.64	115.54
2	A	462	PFA	O9-C14-N6	2.74	126.53	121.49
2	B	463	PFA	C5-C6-C1	2.66	121.79	117.94
2	A	462	PFA	O20-C1-C6	2.47	123.64	118.32
2	A	462	PFA	C8-C25-C24	-2.38	107.60	111.71
2	A	462	PFA	C14-N5-N3	-2.37	121.11	124.17
2	A	462	PFA	C22-C24-C26	2.11	118.87	116.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	463	PFA	C5-C4-N5-C14
2	A	462	PFA	C5-C4-N5-C14
2	B	463	PFA	C3-C4-N5-C14

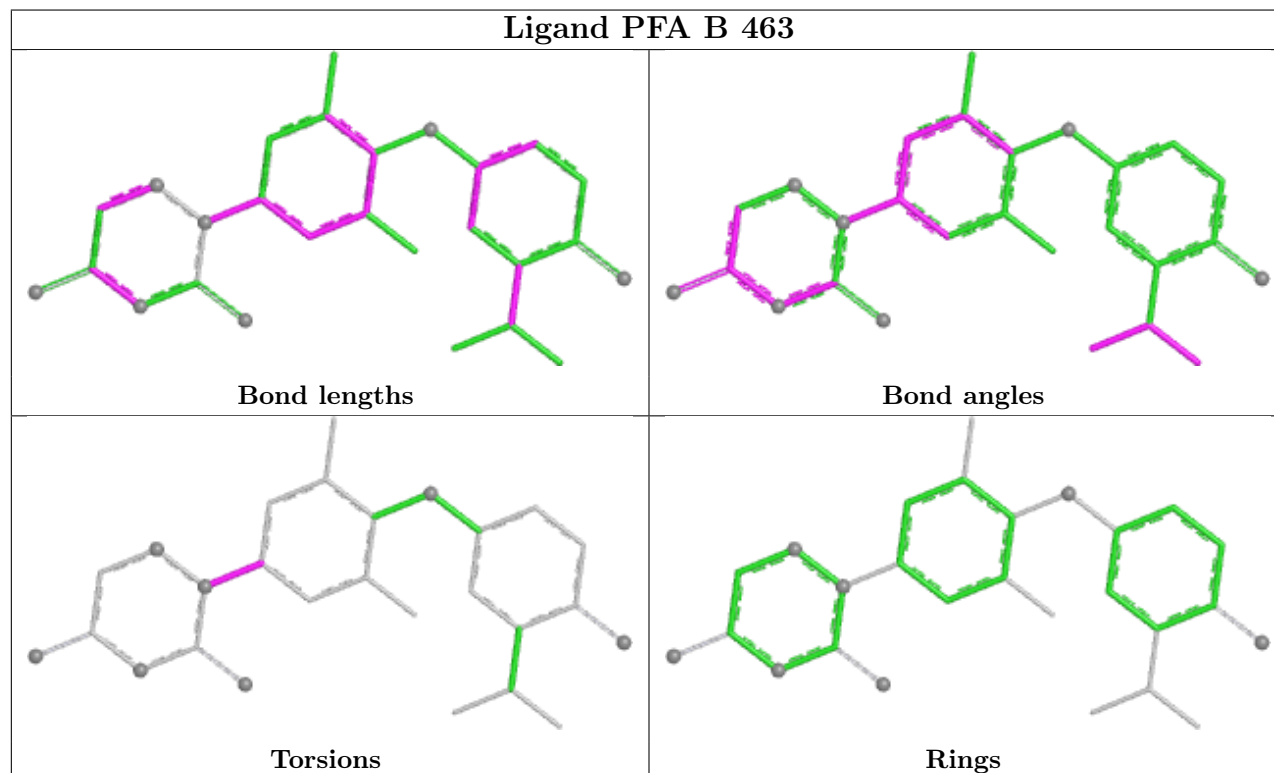
There are no ring outliers.

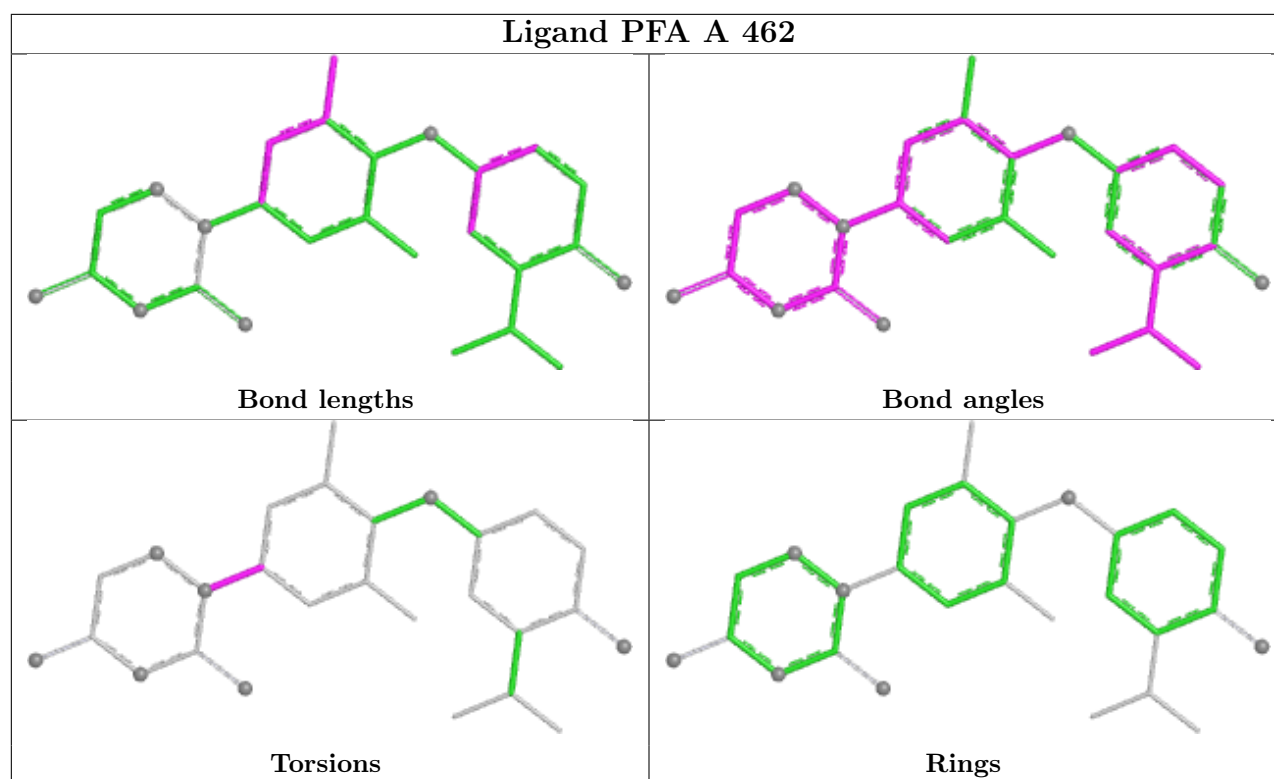
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	463	PFA	6	0
2	A	462	PFA	5	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

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, 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	248/258 (96%)	-0.11	9 (3%) 46 43	13, 23, 46, 109	0
1	B	239/258 (92%)	0.23	11 (4%) 37 34	18, 29, 56, 108	0
All	All	487/516 (94%)	0.06	20 (4%) 41 38	13, 26, 52, 109	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	TRP	6.6
1	A	239	TRP	5.6
1	B	240	LYS	4.0
1	B	409	TYR	4.0
1	A	240	LYS	3.8
1	A	241	GLN	3.4
1	B	461	ASP	3.2
1	A	234	ALA	3.2
1	B	241	GLN	3.1
1	B	235	GLN	3.0
1	B	253	ALA	2.8
1	A	248	GLU	2.7
1	B	223	LYS	2.6
1	B	449	GLU	2.5
1	A	235	GLN	2.5
1	B	250	ILE	2.5
1	A	461	ASP	2.3
1	A	242	LYS	2.3
1	B	242	LYS	2.2
1	A	243	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

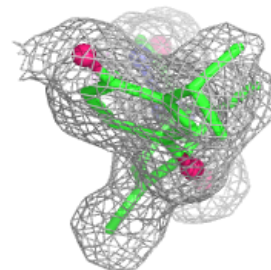
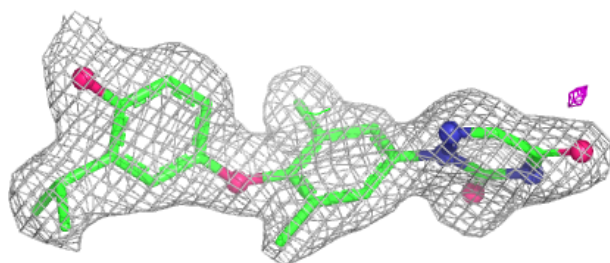
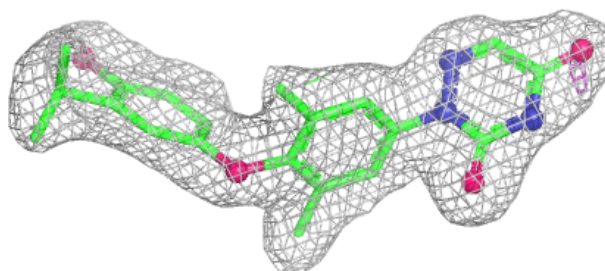
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PFA	B	463	27/27	0.94	0.07	17,25,29,29	0
2	PFA	A	462	27/27	0.96	0.05	10,16,18,19	0

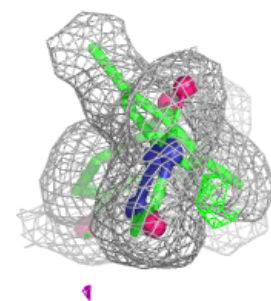
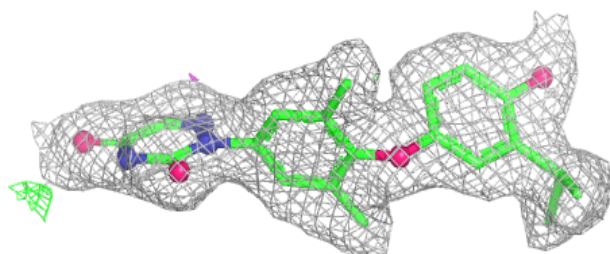
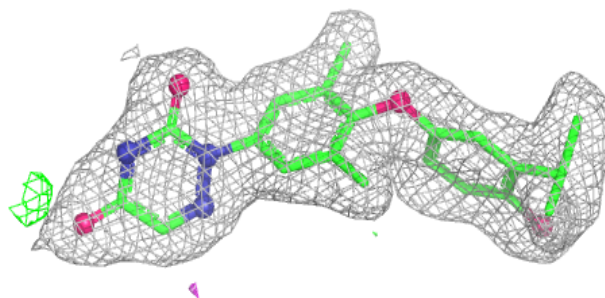
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PFA B 463:

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

**Electron density around PFA A 462:**

$2mF_o-DF_c$ (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.