



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:10 PM UTC

PDB ID : 3TY0 / pdb_00003ty0
Title : Structure of PPARgamma ligand binding domain in complex with (R)-5-(3-((3-(6-methoxybenzo[d]isoxazol-3-yl)-2-oxo-2,3-dihydro-1H-benzo[d]imidazol-1-yl)methyl)phenyl)-5-methyloxazolidine-2,4-dione
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Deposited on : 2011-09-23
Resolution : 2.00 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

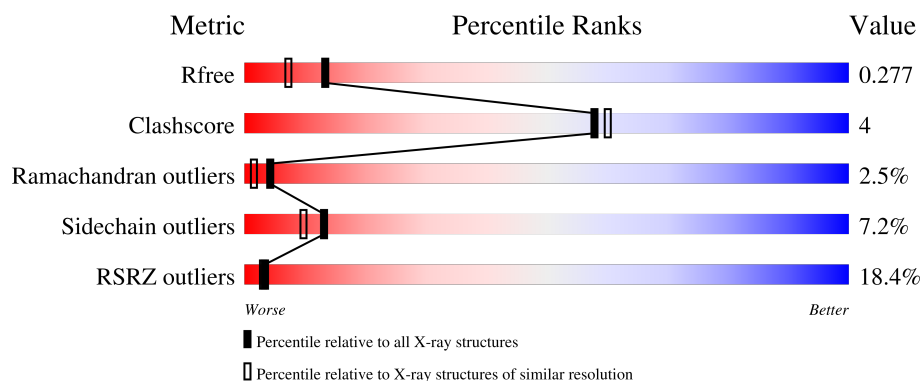
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	277	18% 83% 15% .
1	B	277	18% 77% 20% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4603 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.

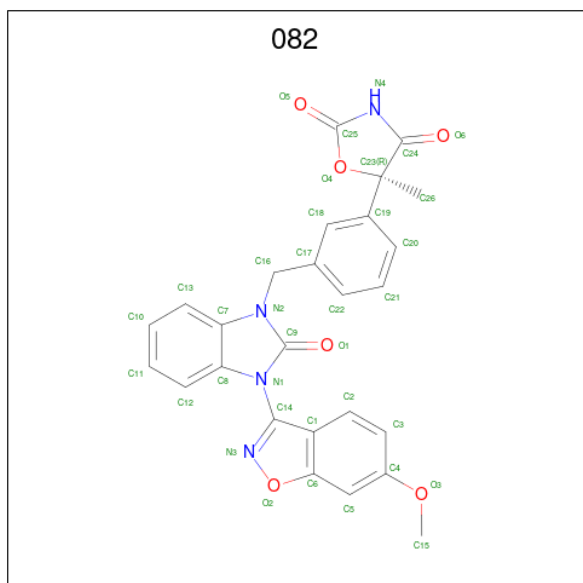
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2220	1431	363	416	10			
1	B	277	Total	C	N	O	S	0	0	0
			2220	1431	363	416	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLY	-	expression tag	UNP P37231
A	202	SER	-	expression tag	UNP P37231
B	701	GLY	-	expression tag	UNP P37231
B	702	SER	-	expression tag	UNP P37231

- Molecule 2 is (5R)-5-(3-{[3-(6-methoxy-1,2-benzoxazol-3-yl)-2-oxo-2,3-dihydro-1H-benzimidazol-1-yl]methyl}phenyl)-5-methyl-1,3-oxazolidine-2,4-dione (CCD ID: 082) (formula: C₂₆H₂₀N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	26	4	6		
2	B	1	Total	C	N	O	0	0
			36	26	4	6		

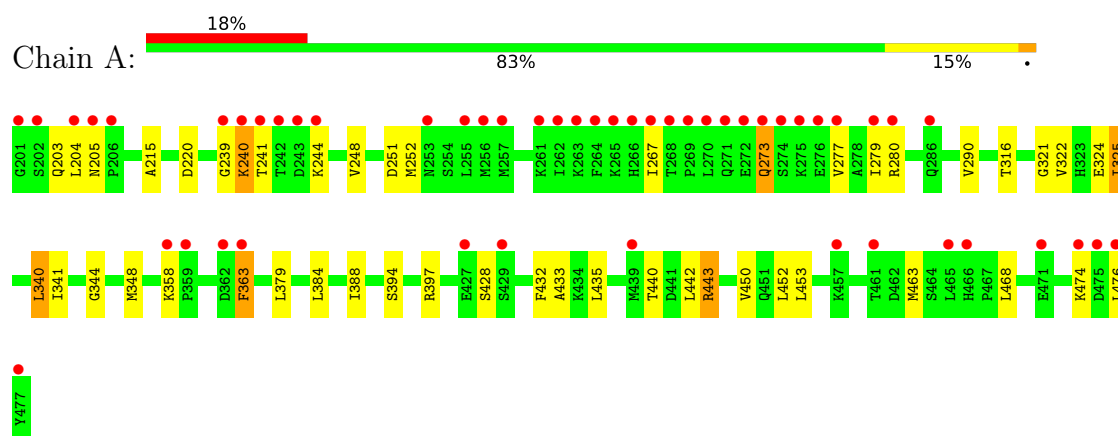
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	47	Total	O	0	0
			47	47		

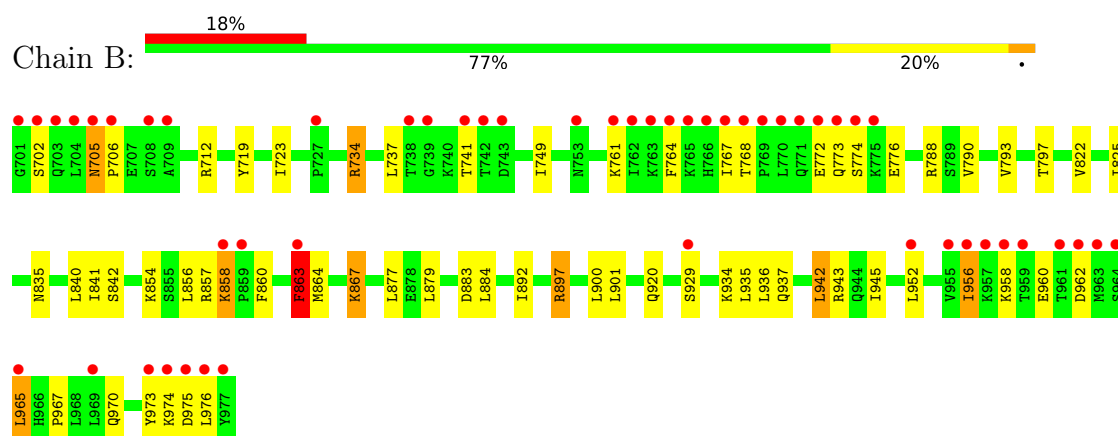
3 Residue-property plots [i](#)

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: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.51Å 61.45Å 119.91Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	37.74 – 2.00 37.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	79.9 (37.74-2.00) 80.1 (37.74-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.00Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.7, BUSTER 2.9.7	Depositor
R, R_{free}	0.234 , 0.273 0.237 , 0.277	Depositor DCC
R_{free} test set	1809 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4603	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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:
082

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	0.85	0/2259	1.40	8/3044 (0.3%)
1	B	0.84	0/2259	1.44	13/3044 (0.4%)
All	All	0.84	0/4518	1.42	21/6088 (0.3%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	863	PHE	CA-CB-CG	5.86	119.66	113.80
1	B	973	TYR	N-CA-C	5.83	119.53	111.55
1	B	835	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	248	VAL	N-CA-C	5.62	116.19	107.99
1	B	822	VAL	N-CA-CB	5.46	116.56	110.51
1	B	856	LEU	CA-C-N	5.43	129.41	121.31
1	B	856	LEU	C-N-CA	5.43	129.41	121.31
1	A	251	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	965	LEU	CA-C-N	5.37	127.85	120.39
1	B	965	LEU	C-N-CA	5.37	127.85	120.39
1	A	363	PHE	CA-CB-CG	5.33	119.13	113.80
1	B	776	GLU	CA-C-N	5.30	127.44	120.60
1	B	776	GLU	C-N-CA	5.30	127.44	120.60
1	B	883	ASP	CA-C-N	5.27	127.34	120.28
1	B	883	ASP	C-N-CA	5.27	127.34	120.28
1	A	239	GLY	CA-C-N	5.14	131.36	121.54
1	A	239	GLY	C-N-CA	5.14	131.36	121.54
1	A	432	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	215	ALA	CA-C-N	5.06	127.02	120.44
1	A	215	ALA	C-N-CA	5.06	127.02	120.44
1	B	860	PHE	N-CA-C	5.02	117.65	111.82

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	2220	0	2281	15	0
1	B	2220	0	2281	27	0
2	A	36	0	20	1	0
2	B	36	0	20	2	0
3	A	44	0	0	0	0
3	B	47	0	0	2	0
All	All	4603	0	4602	41	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 4.

All (41) 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:440:THR:HG21	1:B:943:ARG:HD3	1.48	0.92
1:B:793:VAL:O	1:B:797:THR:HG23	1.84	0.77
1:A:325:ILE:HD13	1:A:388:ILE:HB	1.80	0.63
1:B:790:VAL:HG22	1:B:976:LEU:HB2	1.84	0.59
1:B:773:GLN:HG3	1:B:774:SER:H	1.67	0.59
1:A:450:VAL:HG21	1:A:476:LEU:HD22	1.90	0.54
1:B:864:MET:HA	1:B:864:MET:HE2	1.90	0.54
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.91	0.52
1:B:734:ARG:HH11	1:B:734:ARG:HG2	1.74	0.52
1:B:934:LYS:HA	1:B:937:GLN:HE21	1.74	0.52
1:B:956:ILE:C	1:B:958:LYS:H	2.17	0.52
1:A:240:LYS:HG2	1:A:244:LYS:HD2	1.93	0.50
1:B:734:ARG:NH1	1:B:737:LEU:HD12	2.26	0.50
1:B:825:ILE:HD11	1:B:892:ILE:HG13	1.94	0.50
1:B:864:MET:HE1	2:B:2:082:H2	1.94	0.49
1:B:967:PRO:HA	1:B:970:GLN:HE21	1.77	0.49
1:B:857:ARG:HH22	1:B:960:GLU:CD	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:ARG:HG2	1:B:734:ARG:NH1	2.27	0.49
1:A:290:VAL:HG13	1:A:468:LEU:HD23	1.94	0.49
1:B:879:LEU:HD11	1:B:935:LEU:HD13	1.96	0.47
1:B:863:PHE:CE1	1:B:864:MET:HE3	2.50	0.46
1:A:273:GLN:HE21	1:A:280:ARG:HD2	1.81	0.46
1:A:279:ILE:HG12	1:A:463:MET:HE2	1.98	0.45
1:B:719:TYR:CZ	1:B:723:ILE:HD11	2.53	0.44
1:B:942:LEU:HA	1:B:945:ILE:HD12	2.00	0.44
1:B:797:THR:HG21	3:B:74:HOH:O	2.18	0.44
1:B:864:MET:HE2	1:B:867:LYS:HG3	2.00	0.43
1:B:897:ARG:HD3	3:B:1:HOH:O	2.17	0.43
1:B:712:ARG:HH12	1:B:920:GLN:NE2	2.16	0.43
1:A:252:MET:SD	1:A:277:VAL:HG11	2.58	0.43
2:A:1:082:H5	2:A:1:082:C25	2.49	0.43
1:A:321:GLY:O	1:A:325:ILE:HG13	2.18	0.43
1:B:734:ARG:HH11	1:B:734:ARG:CG	2.32	0.42
1:B:788:ARG:HG3	2:B:2:082:N3	2.35	0.42
1:A:324:GLU:OE2	1:A:443:ARG:HD2	2.19	0.42
1:A:340:LEU:HG	1:A:344:GLY:HA2	2.01	0.42
1:B:749:ILE:HD11	1:B:764:PHE:CZ	2.55	0.42
1:A:341:ILE:HD13	1:A:348:MET:HE3	2.02	0.41
1:A:394:SER:O	1:A:397:ARG:HG2	2.21	0.41
1:A:433:ALA:HA	1:B:936:LEU:HD13	2.02	0.41
1:B:705:ASN:H	1:B:706:PRO:HA	1.86	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	275/277 (99%)	251 (91%)	19 (7%)	5 (2%)	6 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	275/277 (99%)	247 (90%)	19 (7%)	9 (3%)	3	1
All	All	550/554 (99%)	498 (90%)	38 (7%)	14 (2%)	4	1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	LYS
1	A	358	LYS
1	A	474	LYS
1	B	858	LYS
1	B	965	LEU
1	B	705	ASN
1	B	741	THR
1	B	842	SER
1	B	929	SER
1	B	962	ASP
1	A	205	ASN
1	B	761	LYS
1	A	273	GLN
1	B	975	ASP

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	249/249 (100%)	233 (94%)	16 (6%)	16	12
1	B	249/249 (100%)	229 (92%)	20 (8%)	11	8
All	All	498/498 (100%)	462 (93%)	36 (7%)	13	10

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
1	A	204	LEU

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Mol	Chain	Res	Type
1	A	220	ASP
1	A	241	THR
1	A	267	ILE
1	A	316	THR
1	A	322	VAL
1	A	325	ILE
1	A	340	LEU
1	A	363	PHE
1	A	384	LEU
1	A	428	SER
1	A	442	LEU
1	A	443	ARG
1	A	452	LEU
1	A	453	LEU
1	B	702	SER
1	B	734	ARG
1	B	767	ILE
1	B	768	THR
1	B	772	GLU
1	B	840	LEU
1	B	841	ILE
1	B	854	LYS
1	B	858	LYS
1	B	863	PHE
1	B	867	LYS
1	B	877	LEU
1	B	884	LEU
1	B	897	ARG
1	B	900	LEU
1	B	901	LEU
1	B	942	LEU
1	B	952	LEU
1	B	956	ILE
1	B	974	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	273	GLN
1	A	283	GLN
1	A	314	GLN

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Mol	Chain	Res	Type
1	A	412	ASN
1	A	424	ASN
1	A	454	GLN
1	B	705	ASN
1	B	786	GLN
1	B	808	ASN
1	B	814	GLN
1	B	920	GLN
1	B	930	GLN
1	B	937	GLN

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	082	A	1	-	40,41,41	1.46	4 (10%)	46,62,62	1.93	11 (23%)
2	082	B	2	-	40,41,41	1.46	4 (10%)	46,62,62	1.91	11 (23%)

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	082	A	1	-	-	0/13/31/31	0/6/6/6
2	082	B	2	-	-	2/13/31/31	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	082	O4-C23	-4.71	1.41	1.47
2	B	2	082	O4-C23	-4.64	1.42	1.47
2	B	2	082	C14-N3	4.18	1.34	1.29
2	A	1	082	C14-N3	3.94	1.34	1.29
2	A	1	082	O2-N3	-3.92	1.39	1.43
2	B	2	082	O2-N3	-3.70	1.39	1.43
2	B	2	082	C24-N4	-2.85	1.32	1.37
2	A	1	082	C24-N4	-2.80	1.32	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	082	O4-C23-C26	7.42	116.31	106.54
2	B	2	082	O4-C23-C26	6.07	114.54	106.54
2	B	2	082	C15-O3-C4	-5.77	105.13	117.50
2	A	1	082	C15-O3-C4	-4.56	107.72	117.50
2	A	1	082	C6-O2-N3	4.34	109.70	107.48
2	B	2	082	C6-O2-N3	4.01	109.53	107.48
2	A	1	082	C23-C24-N4	3.92	109.74	107.25
2	B	2	082	C23-C24-N4	3.63	109.55	107.25
2	A	1	082	C2-C1-C14	3.41	137.06	131.80
2	B	2	082	C6-C5-C4	-3.06	113.89	119.13
2	B	2	082	C2-C1-C14	2.87	136.24	131.80
2	A	1	082	C6-C5-C4	-2.77	114.38	119.13
2	A	1	082	O6-C24-C23	-2.72	123.42	125.73
2	B	2	082	O6-C24-C23	-2.45	123.65	125.73
2	B	2	082	C20-C19-C23	2.44	124.75	120.71
2	B	2	082	C17-C16-N2	-2.44	109.50	113.46
2	B	2	082	C3-C2-C1	-2.42	116.86	120.86
2	A	1	082	C20-C19-C23	2.37	124.64	120.71
2	A	1	082	C3-C2-C1	-2.22	117.19	120.86
2	A	1	082	O5-C25-N4	-2.08	126.27	129.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	082	C2-C3-C4	2.05	122.07	119.73
2	A	1	082	C2-C3-C4	2.02	122.04	119.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

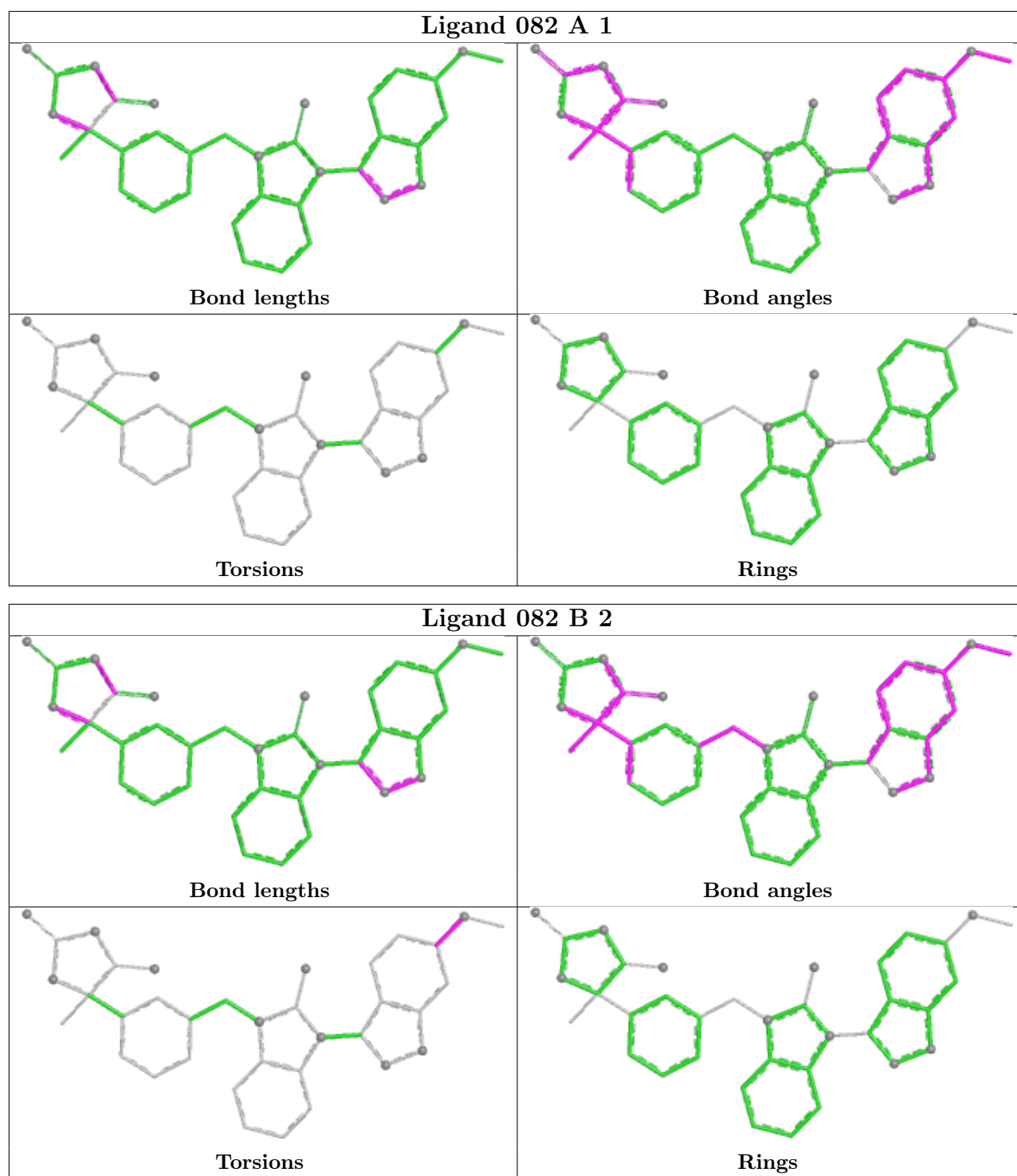
Mol	Chain	Res	Type	Atoms
2	B	2	082	C3-C4-O3-C15
2	B	2	082	C5-C4-O3-C15

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	082	1	0
2	B	2	082	2	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 ⓘ

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, 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	277/277 (100%)	1.02	51 (18%) 3 3	29, 47, 120, 153	0
1	B	277/277 (100%)	1.20	51 (18%) 3 3	28, 46, 109, 150	0
All	All	554/554 (100%)	1.11	102 (18%) 3 3	28, 47, 112, 153	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	976	LEU	8.4
1	B	741	THR	7.8
1	B	769	PRO	7.7
1	B	975	ASP	6.6
1	B	770	LEU	6.5
1	A	266	HIS	6.2
1	A	242	THR	6.2
1	A	241	THR	6.1
1	A	204	LEU	5.8
1	B	977	TYR	5.5
1	B	702	SER	5.2
1	A	362	ASP	5.1
1	A	262	ILE	5.1
1	B	704	LEU	5.1
1	B	964	SER	5.1
1	B	709	ALA	5.0
1	B	708	SER	4.9
1	B	738	THR	4.8
1	B	772	GLU	4.7
1	A	202	SER	4.6
1	B	956	ILE	4.6
1	B	765	LYS	4.5
1	B	767	ILE	4.4
1	B	701	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	255	LEU	4.4
1	B	961	THR	4.3
1	A	359	PRO	4.2
1	A	267	ILE	4.1
1	A	274	SER	4.1
1	B	957	LYS	4.1
1	B	768	THR	4.1
1	A	261	LYS	4.1
1	A	270	LEU	4.0
1	A	273	GLN	4.0
1	B	764	PHE	4.0
1	A	265	LYS	3.9
1	B	955	VAL	3.9
1	B	965	LEU	3.9
1	A	269	PRO	3.8
1	B	963	MET	3.8
1	A	476	LEU	3.6
1	A	240	LYS	3.6
1	A	275	LYS	3.6
1	A	257	MET	3.5
1	B	959	THR	3.5
1	B	705	ASN	3.5
1	A	264	PHE	3.5
1	A	256	MET	3.4
1	B	859	PRO	3.4
1	B	766	HIS	3.4
1	B	743	ASP	3.4
1	A	477	TYR	3.4
1	B	774	SER	3.4
1	A	263	LYS	3.3
1	B	973	TYR	3.3
1	B	974	LYS	3.3
1	A	201	GLY	3.3
1	A	268	THR	3.2
1	B	952	LEU	3.1
1	A	429	SER	3.0
1	B	742	THR	3.0
1	A	206	PRO	3.0
1	B	958	LYS	3.0
1	A	239	GLY	2.9
1	B	706	PRO	2.9
1	A	253	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	474	LYS	2.9
1	B	969	LEU	2.9
1	A	272	GLU	2.8
1	B	771	GLN	2.8
1	A	465	LEU	2.7
1	A	286	GLN	2.7
1	B	762	ILE	2.7
1	B	775	LYS	2.7
1	B	962	ASP	2.7
1	A	277	VAL	2.6
1	A	279	ILE	2.6
1	A	276	GLU	2.6
1	B	761	LYS	2.6
1	A	439	MET	2.5
1	B	703	GLN	2.4
1	B	763	LYS	2.4
1	B	929	SER	2.4
1	A	244	LYS	2.3
1	B	773	GLN	2.3
1	A	205	ASN	2.3
1	A	427	GLU	2.3
1	B	727	PRO	2.3
1	B	753	ASN	2.3
1	A	466	HIS	2.3
1	A	457	LYS	2.3
1	A	363	PHE	2.2
1	B	739	GLY	2.2
1	A	471	GLU	2.2
1	A	461	THR	2.2
1	A	358	LYS	2.2
1	A	243	ASP	2.2
1	A	271	GLN	2.1
1	B	858	LYS	2.1
1	A	475	ASP	2.1
1	B	863	PHE	2.1
1	A	280	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 [i](#)

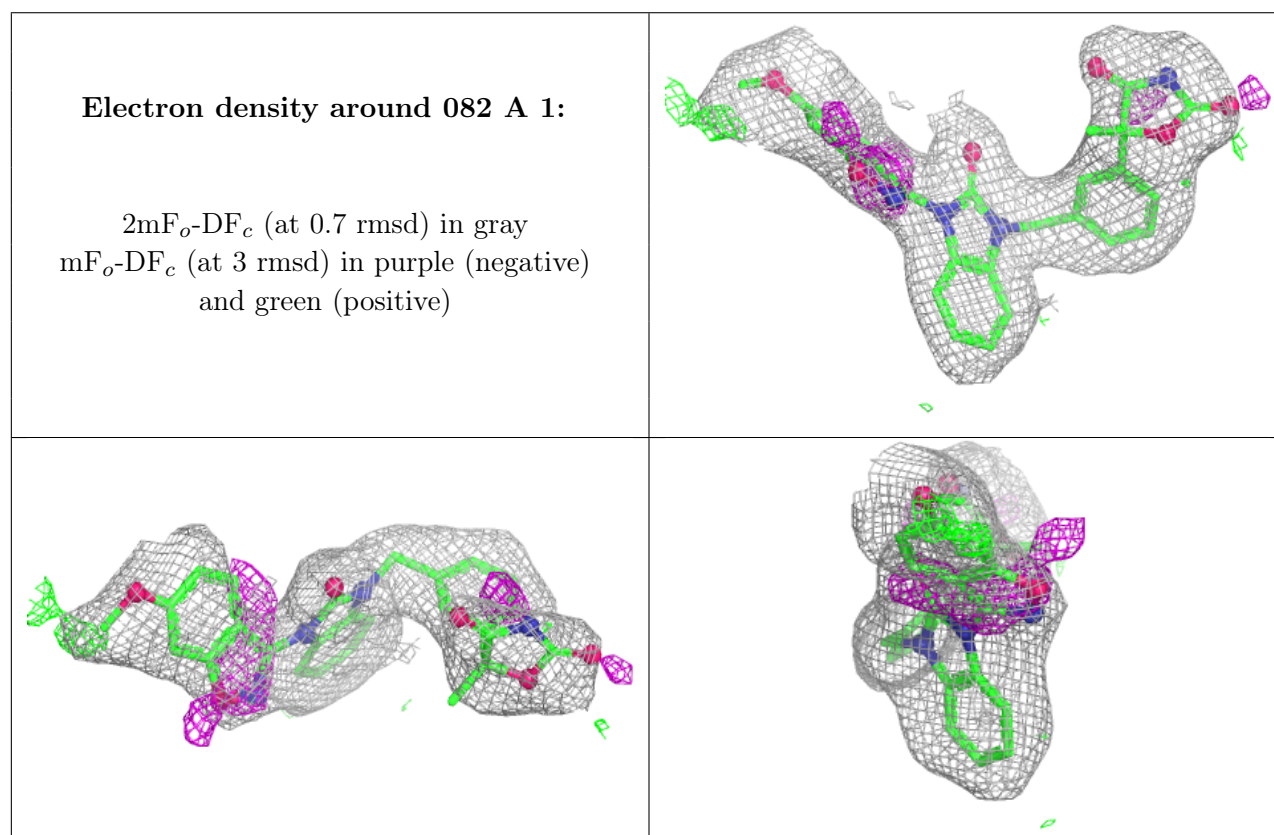
There are no oligosaccharides in this entry.

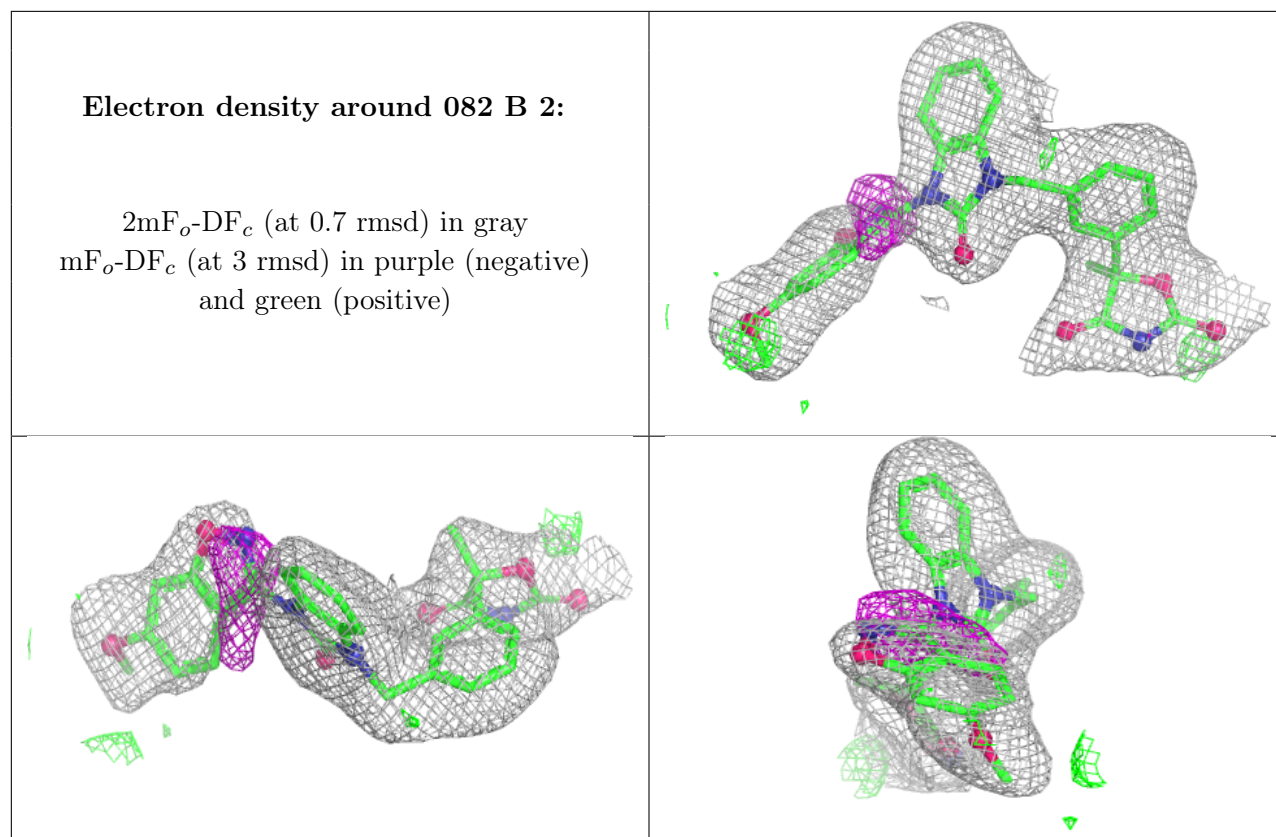
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	082	A	1	36/36	0.81	0.14	46,57,70,72	0
2	082	B	2	36/36	0.85	0.13	44,54,61,66	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 [i](#)

There are no such residues in this entry.