



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:14 am BST

PDB ID : 3TY0
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
Authors : Soisson, S.M.; Meinke, P.M.; McKeever, B.; Liu, W.
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

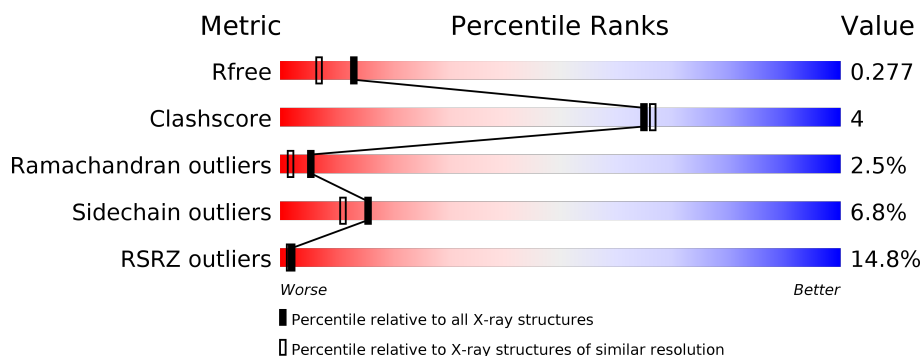
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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	<div> <div>13%</div> <div>86%</div> <div>13%</div> </div>
1	B	277	<div> <div>17%</div> <div>79%</div> <div>18%</div> </div>

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.

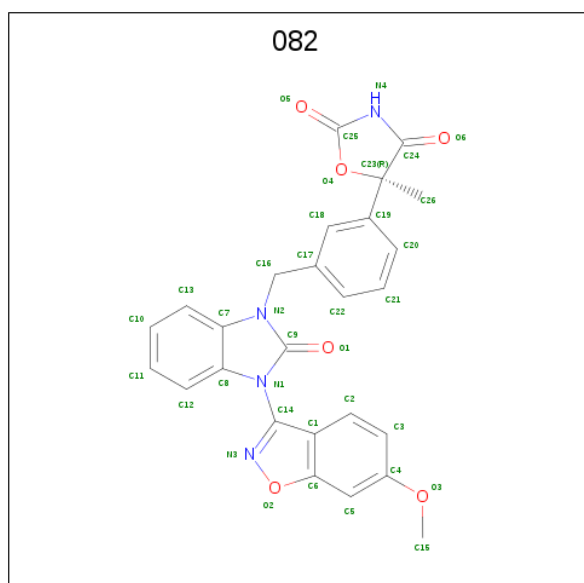
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

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 (three-letter code: 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		

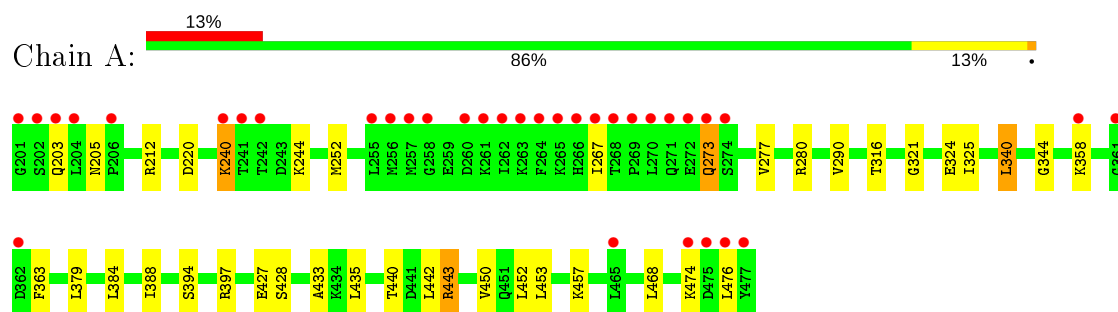
- Molecule 3 is water.

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

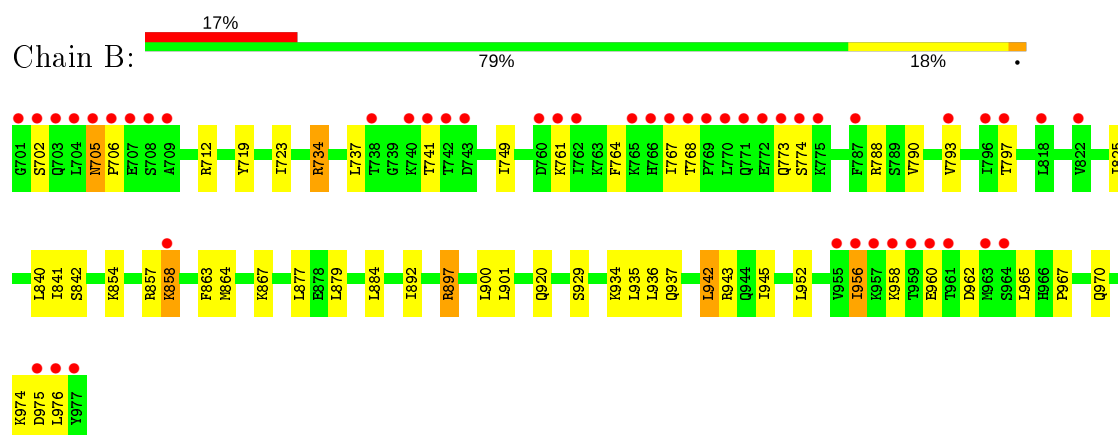
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 45.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	79.9 (37.74-2.00) 80.2 (45.68-2.00)	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)	0.35 , 47.8	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	0.49	0/2259	0.68	0/3044
1	B	0.48	0/2259	0.71	0/3044
All	All	0.48	0/4518	0.69	0/6088

There are no bond length outliers.

There are no bond angle outliers.

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	13	0
1	B	2220	0	2281	25	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	37	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 (37) 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: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:864:MET:HA	1:B:864:MET:HE2	1.91	0.52
1:B:934:LYS:HA	1:B:937:GLN:HE21	1.74	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:967:PRO:HA	1:B:970:GLN:HE21	1.77	0.49
1:B:734:ARG:NH1	1:B:734:ARG:HG2	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:956:ILE:C	1:B:958:LYS:H	2.17	0.47
1:A:273:GLN:HE21	1:A:280:ARG:HD2	1.81	0.46
1:B:857:ARG:HH22	1:B:960:GLU:CD	2.19	0.44
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:897:ARG:HD3	3:B:1:HOH:O	2.17	0.43
1:B:864:MET:HE3	2:B:2:082:H2	1.99	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:C25	2:A:1:082:H5	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: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%)	8	3
1	B	275/277 (99%)	247 (90%)	19 (7%)	9 (3%)	4	1
All	All	550/554 (99%)	498 (90%)	38 (7%)	14 (2%)	5	2

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 [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	249/249 (100%)	234 (94%)	15 (6%)	19	14
1	B	249/249 (100%)	230 (92%)	19 (8%)	13	8
All	All	498/498 (100%)	464 (93%)	34 (7%)	16	11

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
1	A	212	ARG
1	A	220	ASP
1	A	267	ILE
1	A	316	THR
1	A	340	LEU
1	A	363	PHE
1	A	384	LEU
1	A	427	GLU
1	A	428	SER
1	A	442	LEU
1	A	443	ARG
1	A	452	LEU
1	A	453	LEU
1	A	457	LYS
1	B	702	SER
1	B	734	ARG
1	B	767	ILE
1	B	768	THR
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	273	GLN
1	A	314	GLN
1	A	424	ASN
1	A	430	GLN
1	A	454	GLN
1	A	470	GLN
1	B	773	GLN
1	B	783	GLN
1	B	786	GLN
1	B	794	GLN
1	B	814	GLN
1	B	920	GLN
1	B	930	GLN
1	B	937	GLN

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 carbohydrates 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
2	082	B	2	-	33,41,41	1.30	3 (9%)	37,62,62	1.97	12 (32%)
2	082	A	1	-	33,41,41	1.34	4 (12%)	37,62,62	1.81	10 (27%)

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	B	2	-	-	4/12/31/31	0/6/6/6
2	082	A	1	-	-	2/12/31/31	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	082	C14-N1	-4.49	1.39	1.45
2	B	2	082	C14-N1	-4.15	1.39	1.45
2	B	2	082	C24-N4	-2.83	1.32	1.37
2	A	1	082	C24-N4	-2.78	1.32	1.37
2	B	2	082	C1-C6	-2.51	1.38	1.43
2	A	1	082	C1-C6	-2.45	1.38	1.43
2	A	1	082	C16-N2	-2.05	1.44	1.48

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	082	C15-O3-C4	-5.70	105.13	117.51
2	B	2	082	C4-C5-C6	-4.64	113.89	119.13
2	A	1	082	C15-O3-C4	-4.51	107.72	117.51
2	A	1	082	C4-C5-C6	-4.20	114.38	119.13
2	A	1	082	C23-C24-N4	3.62	109.74	107.28
2	B	2	082	C23-C24-N4	3.35	109.55	107.28
2	B	2	082	C3-C2-C1	-3.07	116.86	121.13
2	B	2	082	C5-C6-C1	2.87	125.66	120.04
2	A	1	082	C3-C2-C1	-2.83	117.19	121.13
2	A	1	082	C5-C6-C1	2.80	125.51	120.04
2	A	1	082	O6-C24-C23	-2.72	123.42	125.74
2	A	1	082	C2-C1-C6	-2.62	118.72	120.38
2	B	2	082	O3-C4-C5	-2.60	117.34	124.43
2	B	2	082	C20-C19-C23	2.54	124.75	120.62
2	A	1	082	C20-C19-C23	2.48	124.64	120.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	082	O6-C24-C23	-2.46	123.65	125.74
2	B	2	082	C9-N1-C14	2.36	127.74	124.60
2	A	1	082	C18-C19-C23	-2.28	117.20	120.57
2	A	1	082	O5-C25-N4	-2.26	126.27	129.83
2	B	2	082	C18-C19-C23	-2.23	117.28	120.57
2	B	2	082	C2-C1-C6	-2.19	119.00	120.38
2	B	2	082	C17-C16-N2	-2.01	109.50	112.63

There are no chirality outliers.

All (6) torsion outliers are listed below:

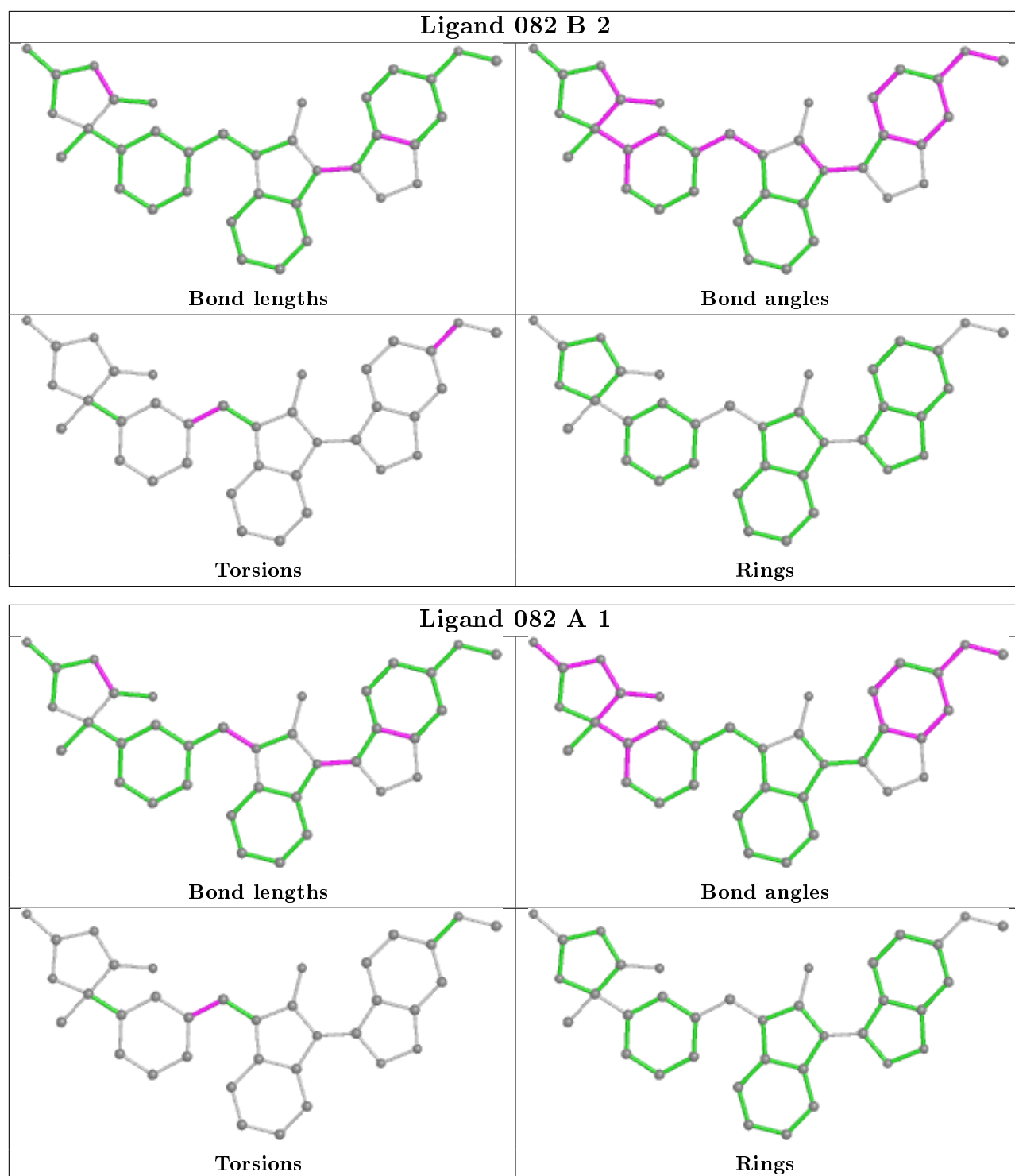
Mol	Chain	Res	Type	Atoms
2	B	2	082	C5-C4-O3-C15
2	B	2	082	C3-C4-O3-C15
2	A	1	082	N2-C16-C17-C18
2	B	2	082	N2-C16-C17-C18
2	A	1	082	N2-C16-C17-C22
2	B	2	082	N2-C16-C17-C22

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

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%)	0.85	35 (12%) 3 3	29, 47, 120, 153	0
1	B	277/277 (100%)	0.97	47 (16%) 1 1	28, 46, 109, 150	0
All	All	554/554 (100%)	0.91	82 (14%) 2 2	28, 47, 112, 153	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	LYS	14.2
1	A	268	THR	12.4
1	A	202	SER	12.1
1	A	267	ILE	12.1
1	B	770	LEU	11.4
1	A	270	LEU	10.1
1	B	769	PRO	9.9
1	A	201	GLY	9.8
1	B	705	ASN	9.7
1	A	269	PRO	9.5
1	B	702	SER	8.9
1	A	274	SER	8.8
1	A	272	GLU	8.5
1	A	262	ILE	8.4
1	B	964	SER	8.3
1	B	976	LEU	7.9
1	B	704	LEU	7.9
1	B	743	ASP	7.9
1	B	741	THR	7.7
1	A	261	LYS	7.4
1	A	265	LYS	7.1
1	A	273	GLN	6.9
1	B	703	GLN	6.4
1	A	204	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	362	ASP	6.1
1	B	742	THR	6.0
1	B	706	PRO	5.8
1	A	241	THR	5.8
1	A	266	HIS	5.6
1	B	977	TYR	5.5
1	B	963	MET	5.5
1	A	203	GLN	5.3
1	B	771	GLN	5.2
1	B	707	GLU	5.1
1	A	271	GLN	5.0
1	B	701	GLY	5.0
1	B	772	GLU	5.0
1	B	858	LYS	4.9
1	A	264	PHE	4.7
1	A	206	PRO	4.6
1	B	975	ASP	4.5
1	B	957	LYS	4.2
1	B	708	SER	4.1
1	B	768	THR	3.9
1	A	465	LEU	3.8
1	B	956	ILE	3.8
1	B	773	GLN	3.7
1	A	242	THR	3.7
1	B	774	SER	3.4
1	A	260	ASP	3.3
1	B	765	LYS	3.3
1	B	766	HIS	3.2
1	A	361	GLY	3.2
1	B	709	ALA	3.0
1	B	767	ILE	3.0
1	B	796	ILE	3.0
1	B	818	LEU	3.0
1	A	474	LYS	2.8
1	A	358	LYS	2.8
1	A	258	GLY	2.7
1	A	475	ASP	2.7
1	B	961	THR	2.7
1	B	760	ASP	2.7
1	A	257	MET	2.6
1	A	477	TYR	2.5
1	B	775	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	793	VAL	2.3
1	B	822	VAL	2.3
1	A	476	LEU	2.3
1	B	955	VAL	2.3
1	B	958	LYS	2.3
1	B	960	GLU	2.3
1	B	959	THR	2.2
1	B	738	THR	2.2
1	A	240	LYS	2.2
1	A	255	LEU	2.1
1	B	761	LYS	2.1
1	A	256	MET	2.1
1	B	740	LYS	2.1
1	B	762	ILE	2.1
1	B	797	THR	2.1
1	B	787	PHE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

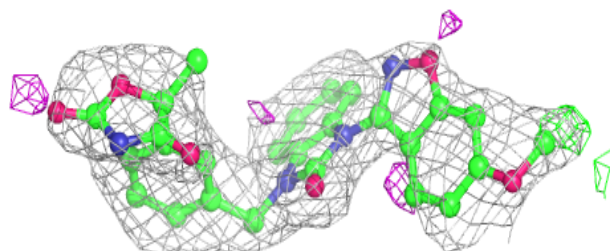
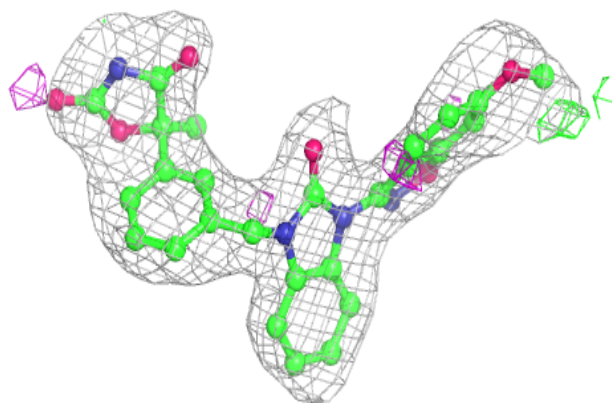
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	082	A	1	36/36	0.85	0.16	46,57,70,72	0
2	082	B	2	36/36	0.86	0.16	44,54,61,66	0

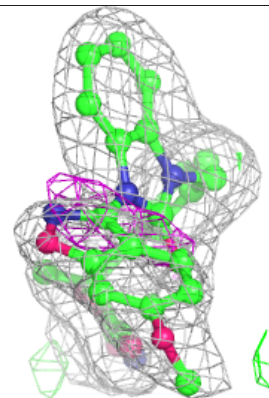
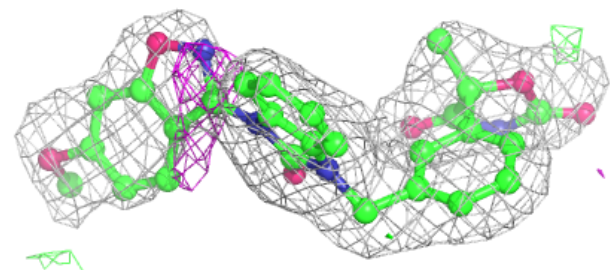
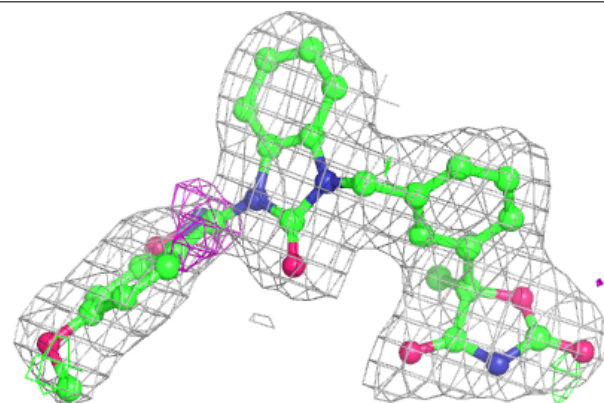
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 082 A 1:

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

**Electron density around 082 B 2:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.