



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:40 PM UTC

PDB ID : 8B90 / pdb_00008b90
Title : Crystal structure of PPARG and NCOR2 with an inverse agonist (compound 7d)
Authors : Friberg, A.; Orsi, D.L.; Pook, E.; Siegel, S.; Lemke, C.T.; Stellfeld, T.; Puetter, V.; Goldstein, J.
Deposited on : 2022-10-05
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

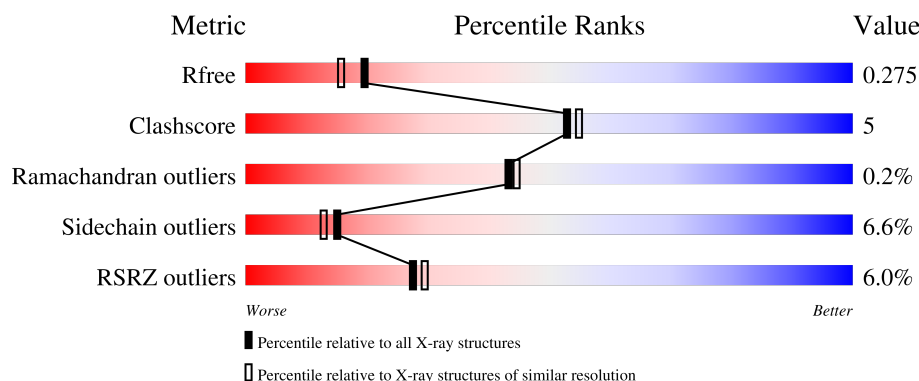
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	279	3% 78% 13% 7%
1	B	279	6% 71% 11% 16%
2	C	23	17% 39% 9% 52%
2	D	23	9% 39% 9% 48%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4248 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	259	Total	C	N	O	S	0	2	0
			2085	1342	343	389	11			
1	B	234	Total	C	N	O	S	0	0	0
			1863	1202	305	347	9			

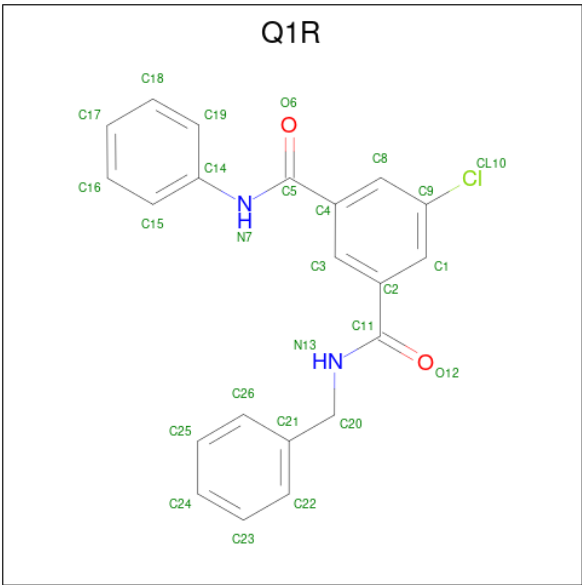
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	expression tag	UNP P37231
A	200	SER	-	expression tag	UNP P37231
A	201	HIS	-	expression tag	UNP P37231
A	202	MET	-	expression tag	UNP P37231
B	199	GLY	-	expression tag	UNP P37231
B	200	SER	-	expression tag	UNP P37231
B	201	HIS	-	expression tag	UNP P37231
B	202	MET	-	expression tag	UNP P37231

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	S	0	0	0
			83	54	15	13	1			
2	D	12	Total	C	N	O	S	0	0	0
			87	56	16	14	1			

- Molecule 3 is 5-chloranyl- {N}3-phenyl- {N}1-(phenylmethyl)benzene-1,3-dicarboxamide (CCD ID: Q1R) (formula: C₂₁H₁₇ClN₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		

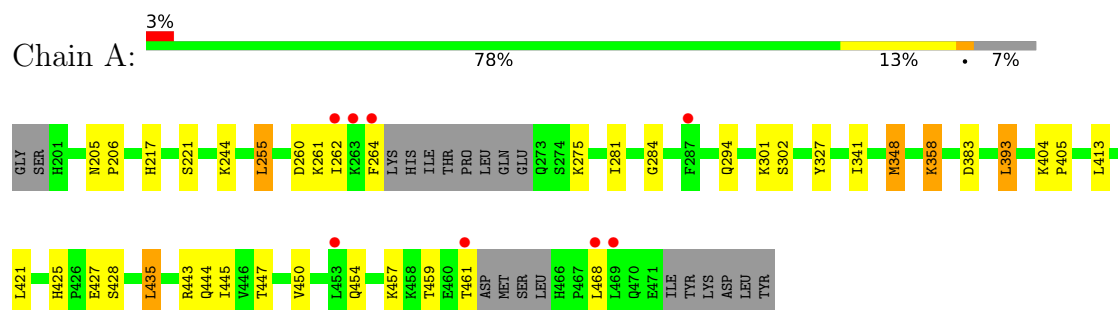
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	29	Total	O	0	0
			29	29		

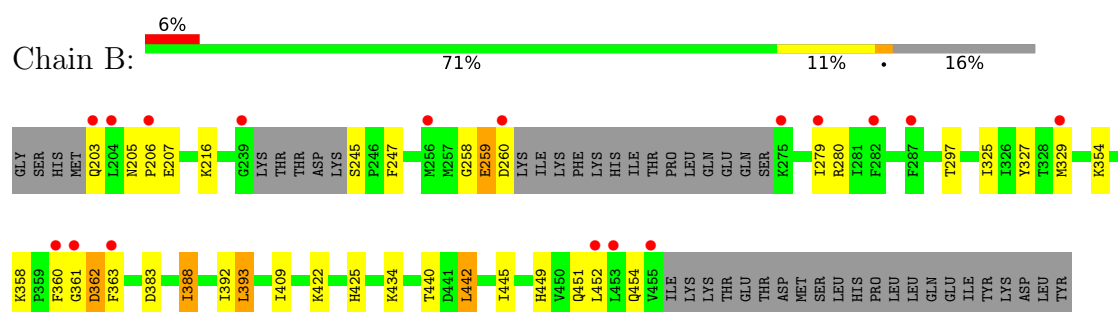
3 Residue-property plots [i](#)

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.

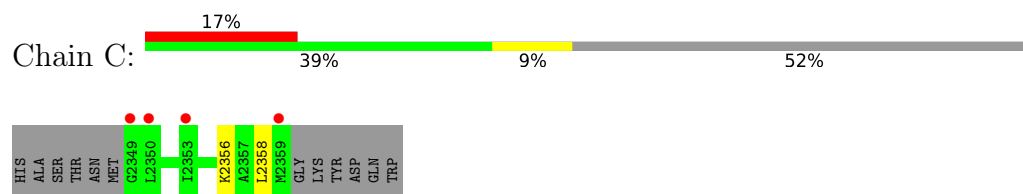
- Molecule 1: Peroxisome proliferator-activated receptor gamma



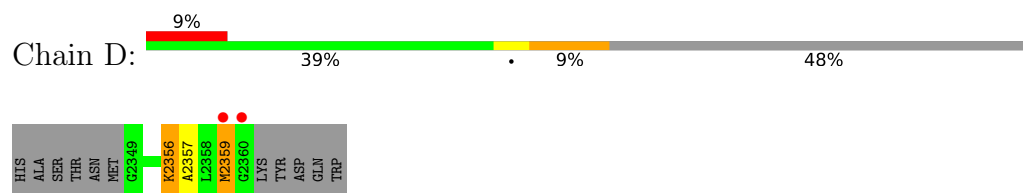
- Molecule 1: Peroxisome proliferator-activated receptor gamma



- Molecule 2: Nuclear receptor corepressor 2



- Molecule 2: Nuclear receptor corepressor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.73Å 85.56Å 120.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.37 – 2.10 45.37 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.37-2.10) 99.9 (45.37-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.274 0.217 , 0.275	Depositor DCC
R_{free} test set	1815 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4248	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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: Q1R

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	1.04	0/2119	1.42	0/2853
1	B	1.02	0/1893	1.44	0/2551
2	C	1.05	0/82	1.61	0/107
2	D	1.17	0/86	1.68	0/112
All	All	1.04	0/4180	1.44	0/5623

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	2085	0	2131	23	0
1	B	1863	0	1905	18	0
2	C	83	0	97	1	0
2	D	87	0	100	3	0
3	A	26	0	0	1	0
4	A	75	0	0	1	0
4	B	29	0	0	0	0
All	All	4248	0	4233	42	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 5.

All (42) 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:B:329:MET:HE3	1:B:388:ILE:HG13	1.47	0.96
1:B:259:GLU:OE1	1:B:280:ARG:NH1	2.21	0.74
1:A:383:ASP:OD2	1:A:425:HIS:HE1	1.78	0.67
1:B:362:ASP:N	1:B:362:ASP:OD1	2.29	0.65
1:B:327:TYR:OH	1:B:449:HIS:CD2	2.52	0.62
1:B:329:MET:CE	1:B:388:ILE:HG13	2.28	0.61
1:B:383:ASP:OD2	1:B:425:HIS:HE1	1.83	0.61
1:A:294:GLN:HE22	1:A:468:LEU:HD22	1.64	0.61
1:A:217:HIS:HE1	1:A:302:SER:O	1.84	0.60
1:A:205:ASN:HB2	1:A:206:PRO:HD2	1.86	0.57
1:A:262:ILE:HG21	1:A:264:PHE:CE1	2.40	0.56
1:B:258:GLY:C	1:B:260:ASP:H	2.16	0.54
2:D:2359:MET:HE3	2:D:2359:MET:HA	1.90	0.54
1:B:393:LEU:HD22	1:B:409:ILE:HB	1.91	0.52
1:B:205:ASN:HB2	1:B:206:PRO:HD2	1.91	0.52
1:A:255:LEU:CD1	1:A:281:ILE:HD11	2.40	0.51
1:A:294:GLN:NE2	1:A:468:LEU:CD2	2.74	0.51
1:A:341:ILE:HD13	1:A:348:MET:CE	2.41	0.51
1:A:425:HIS:HD2	1:A:427:GLU:OE2	1.97	0.48
1:A:255:LEU:HD13	1:A:281:ILE:HD11	1.96	0.48
1:A:294:GLN:NE2	1:A:468:LEU:HD22	2.28	0.47
1:A:404:LYS:N	1:A:405:PRO:HD2	2.30	0.46
1:B:297:THR:HG21	2:D:2357:ALA:HB3	1.99	0.45
1:A:348:MET:HE2	1:A:348:MET:HB2	1.92	0.45
1:B:247:PHE:C	1:B:247:PHE:CD1	2.95	0.45
1:A:284:GLY:HA3	3:A:1001:Q1R:C20	2.47	0.45
1:A:444:GLN:O	1:A:447:THR:HB	2.17	0.44
2:D:2356:LYS:HD3	2:D:2356:LYS:C	2.42	0.44
1:B:325:ILE:HD11	1:B:392:ILE:HG13	2.00	0.43
1:B:360:PHE:O	1:B:363:PHE:HD2	2.01	0.43
1:A:327:TYR:CE2	1:A:445:ILE:CG2	3.02	0.43
1:A:443:ARG:NH1	1:B:440:THR:HG21	2.34	0.42
1:B:258:GLY:C	1:B:260:ASP:N	2.78	0.42
1:B:442:LEU:HD12	1:B:442:LEU:HA	1.91	0.42
1:A:221:SER:OG	1:A:302:SER:OG	2.31	0.42
1:A:301:LYS:HE2	2:C:2358:LEU:HA	2.02	0.41
1:A:421:LEU:HD11	1:A:435:LEU:HD22	2.01	0.41
1:A:358:LYS:NZ	4:A:1101:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:GLN:O	1:B:454:GLN:HB2	2.20	0.41
1:A:260:ASP:HB3	1:A:261:LYS:HD2	2.02	0.41
1:B:354:LYS:HA	1:B:361:GLY:O	2.21	0.41
1:A:393:LEU:HD13	1:A:413:LEU:HD11	2.02	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	255/279 (91%)	247 (97%)	8 (3%)	0	100	100
1	B	228/279 (82%)	222 (97%)	5 (2%)	1 (0%)	30	28
2	C	9/23 (39%)	9 (100%)	0	0	100	100
2	D	10/23 (44%)	10 (100%)	0	0	100	100
All	All	502/604 (83%)	488 (97%)	13 (3%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLU

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	233/251 (93%)	220 (94%)	13 (6%)	19	18
1	B	207/251 (82%)	193 (93%)	14 (7%)	14	12
2	C	8/18 (44%)	7 (88%)	1 (12%)	4	2
2	D	8/18 (44%)	6 (75%)	2 (25%)	0	0
All	All	456/538 (85%)	426 (93%)	30 (7%)	15	13

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
1	A	255	LEU
1	A	275	LYS
1	A	348	MET
1	A	358	LYS
1	A	393	LEU
1	A	428	SER
1	A	435	LEU
1	A	450	VAL
1	A	454	GLN
1	A	457	LYS
1	A	459	THR
1	A	461	THR
1	B	203	GLN
1	B	207	GLU
1	B	216	LYS
1	B	245	SER
1	B	279	ILE
1	B	358	LYS
1	B	362	ASP
1	B	388	ILE
1	B	393	LEU
1	B	422	LYS
1	B	434	LYS
1	B	442	LEU
1	B	445	ILE
1	B	452	LEU
2	C	2356	LYS
2	D	2356	LYS
2	D	2359	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	HIS
1	A	294	GLN
1	A	425	HIS
1	A	454	GLN
1	B	253	ASN
1	B	415	GLN
1	B	425	HIS
1	B	449	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](#)

1 ligand is 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	Q1R	A	1001	-	28,28,28	0.88	1 (3%)	37,37,37	1.08	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	Q1R	A	1001	-	-	0/17/17/17	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	Q1R	C14-N7	-3.05	1.35	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	Q1R	C4-C8-C9	-2.40	116.59	119.17
3	A	1001	Q1R	C18-C19-C14	2.28	122.36	119.73
3	A	1001	Q1R	C26-C21-C22	2.10	121.35	118.23
3	A	1001	Q1R	O6-C5-C4	-2.09	116.77	120.90

There are no chirality outliers.

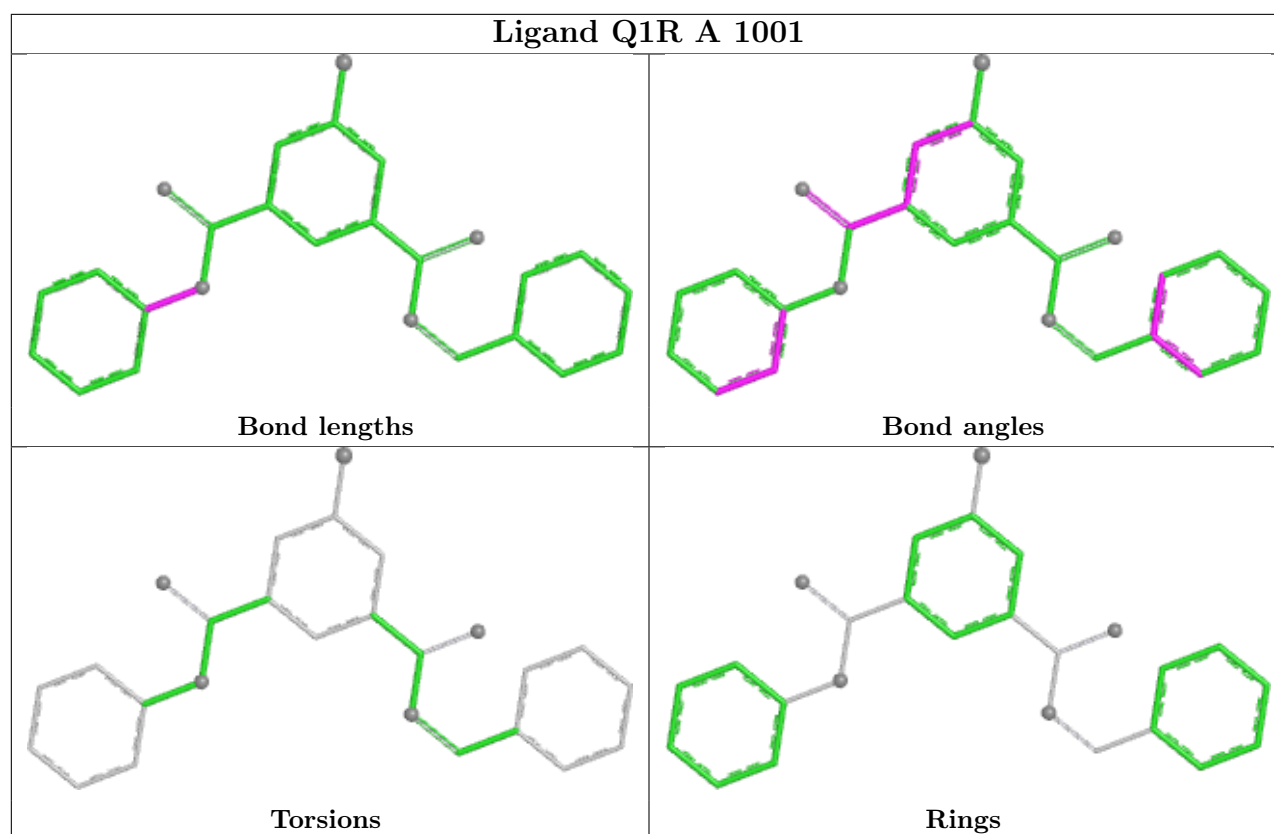
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	Q1R	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 [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	259/279 (92%)	0.34	8 (3%) 51 54	18, 42, 85, 112	2 (0%)
1	B	234/279 (83%)	0.47	17 (7%) 21 22	28, 47, 82, 100	0
2	C	11/23 (47%)	1.26	4 (36%) 1 1	50, 64, 84, 93	0
2	D	12/23 (52%)	1.23	2 (16%) 4 4	51, 61, 82, 89	0
All	All	516/604 (85%)	0.44	31 (6%) 27 29	18, 45, 83, 112	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	455	VAL	5.7
1	A	264	PHE	4.2
1	A	263	LYS	3.8
1	A	262	ILE	3.6
1	B	239	GLY	3.6
1	A	469	LEU	3.3
1	B	282	PHE	3.1
1	B	275	LYS	3.0
2	C	2359	MET	3.0
2	D	2359	MET	3.0
1	A	461	THR	2.9
1	B	287	PHE	2.9
1	B	204	LEU	2.8
1	B	206	PRO	2.7
1	B	279	ILE	2.5
1	B	452	LEU	2.5
2	C	2350	LEU	2.4
1	A	468	LEU	2.4
1	B	256	MET	2.3
1	A	287	PHE	2.2
1	B	361	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	2349	GLY	2.2
1	A	453	LEU	2.2
2	D	2360	GLY	2.1
1	B	260	ASP	2.1
2	C	2353	ILE	2.1
1	B	360	PHE	2.1
1	B	329	MET	2.0
1	B	453	LEU	2.0
1	B	363	PHE	2.0
1	B	203	GLN	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](#)

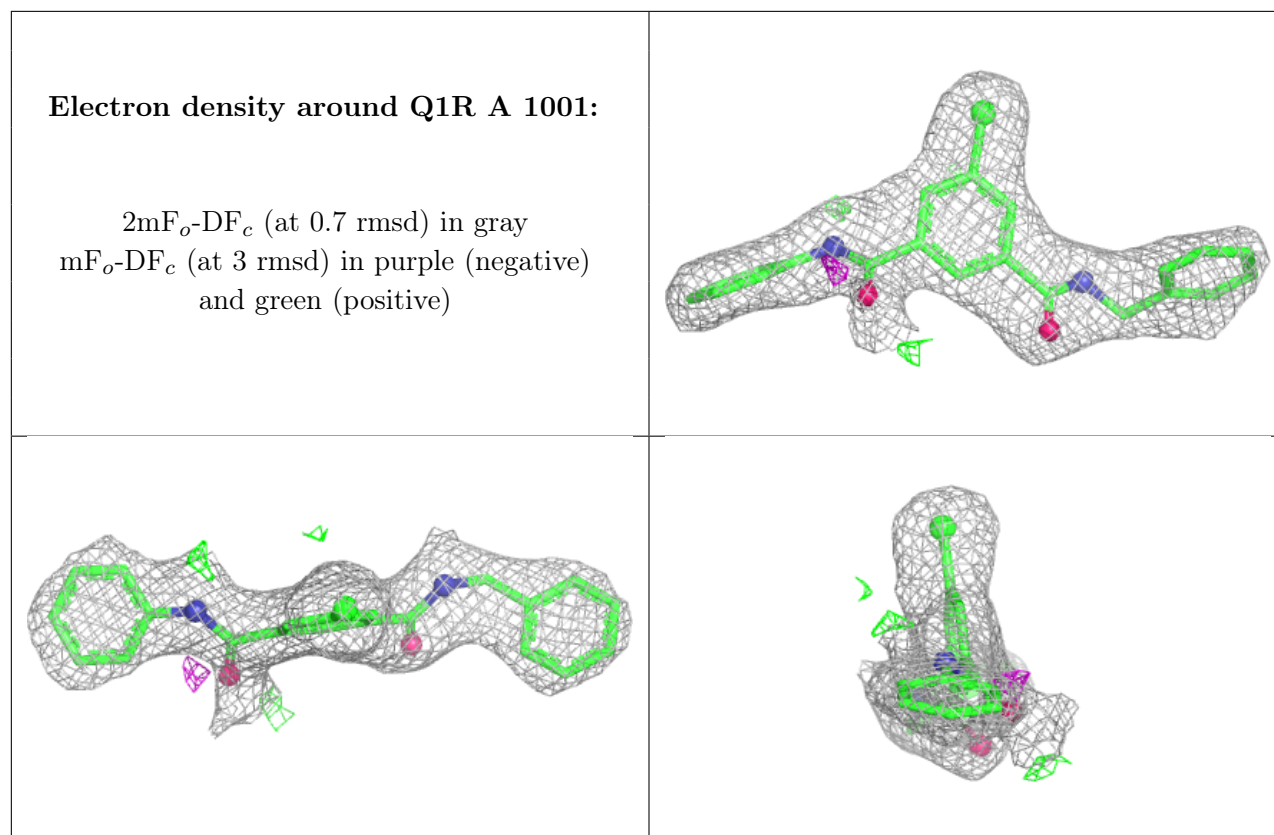
There are no oligosaccharides in this entry.

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, 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
3	Q1R	A	1001	26/26	0.91	0.12	54,60,65,68	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.