



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 01:25 PM EDT

PDB ID : 7SQA  
Title : PPAR gamma LBD bound to SR10221 and SMRT corepressor motif  
Authors : Frkic, R.L.; Pederick, J.L.; Bruning, J.B.  
Deposited on : 2021-11-05  
Resolution : 2.50 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](mailto: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>.

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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 : 2.36  
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) : 2.36

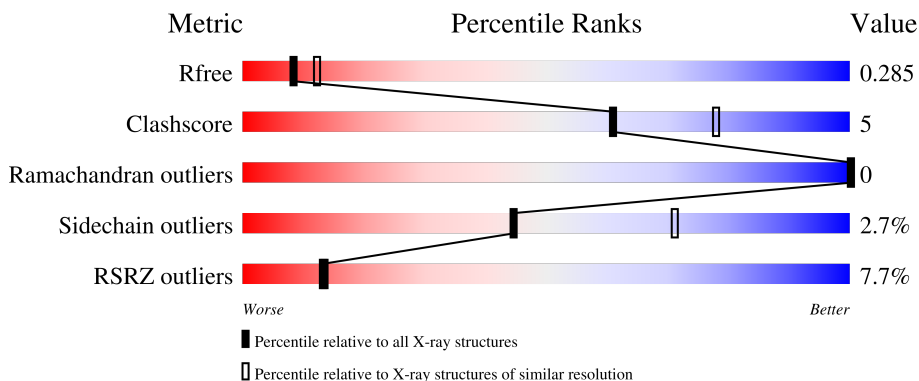
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	290	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div>
1	B	290	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>
2	C	22	<div style="display: flex; align-items: center;"> <div style="width: 23%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: grey;"></div> </div>
2	D	22	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: grey;"></div> </div>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4570 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
			Total	C	N	O	S			
1	A	259	2063	1329	341	383	10	0	0	0
1	B	256	2033	1310	333	380	10	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	MET	-	initiating methionine	UNP P37231
A	189	ALA	-	expression tag	UNP P37231
A	190	HIS	-	expression tag	UNP P37231
A	191	HIS	-	expression tag	UNP P37231
A	192	HIS	-	expression tag	UNP P37231
A	193	HIS	-	expression tag	UNP P37231
A	194	HIS	-	expression tag	UNP P37231
A	195	HIS	-	expression tag	UNP P37231
A	196	VAL	-	expression tag	UNP P37231
A	197	ASP	-	expression tag	UNP P37231
A	198	ASP	-	expression tag	UNP P37231
A	199	ASP	-	expression tag	UNP P37231
A	200	ASP	-	expression tag	UNP P37231
A	201	LYS	-	expression tag	UNP P37231
A	202	MET	-	expression tag	UNP P37231
B	188	MET	-	initiating methionine	UNP P37231
B	189	ALA	-	expression tag	UNP P37231
B	190	HIS	-	expression tag	UNP P37231
B	191	HIS	-	expression tag	UNP P37231
B	192	HIS	-	expression tag	UNP P37231
B	193	HIS	-	expression tag	UNP P37231
B	194	HIS	-	expression tag	UNP P37231
B	195	HIS	-	expression tag	UNP P37231
B	196	VAL	-	expression tag	UNP P37231
B	197	ASP	-	expression tag	UNP P37231

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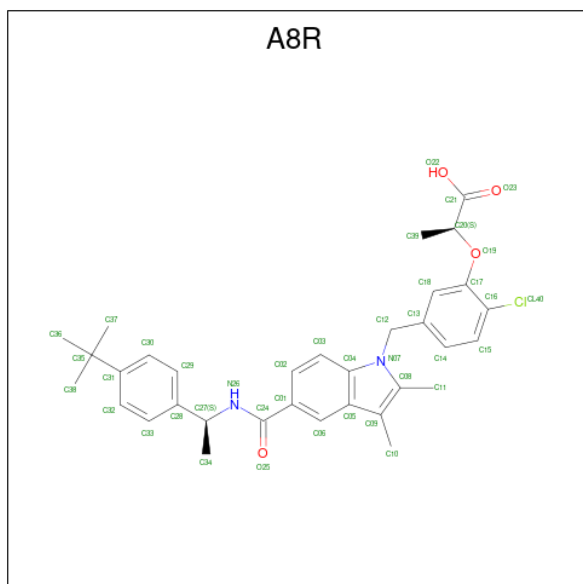
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Chain	Residue	Modelled	Actual	Comment	Reference
B	198	ASP	-	expression tag	UNP P37231
B	199	ASP	-	expression tag	UNP P37231
B	200	ASP	-	expression tag	UNP P37231
B	201	LYS	-	expression tag	UNP P37231
B	202	MET	-	expression tag	UNP P37231

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	S	0	0	0
			112	71	21	18	2			
2	D	12	Total	C	N	O	S	0	0	0
			91	59	16	14	2			

- Molecule 3 is (2S)-2-{5-[(5-[(1S)-1-(4-tert-butylphenyl)ethyl]carbamoyl)-2,3-dimethyl-1H-indol-1-yl)methyl]-2-chlorophenoxy}propanoic acid (three-letter code: A8R) (formula: C<sub>33</sub>H<sub>37</sub>ClN<sub>2</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			40	33	1	2	4		
3	B	1	Total	C	Cl	N	O	0	0
			40	33	1	2	4		

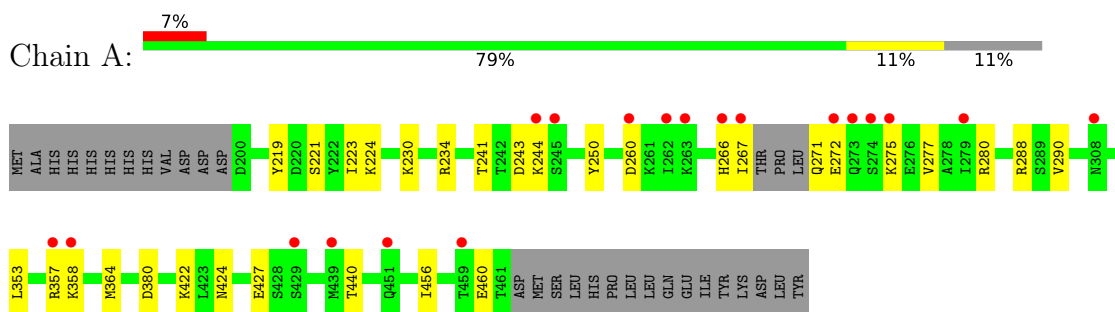
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	106	Total 106	O 106	0	0
4	B	76	Total 76	O 76	0	0
4	C	5	Total 5	O 5	0	0
4	D	4	Total 4	O 4	0	0

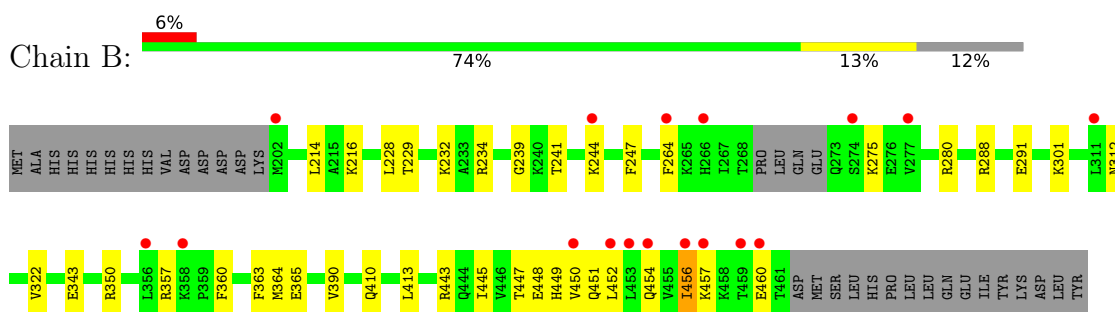
### 3 Residue-property plots [i](#)

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.

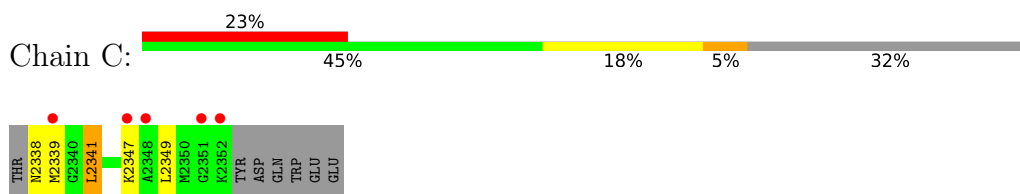
- Molecule 1: Peroxisome proliferator-activated receptor gamma



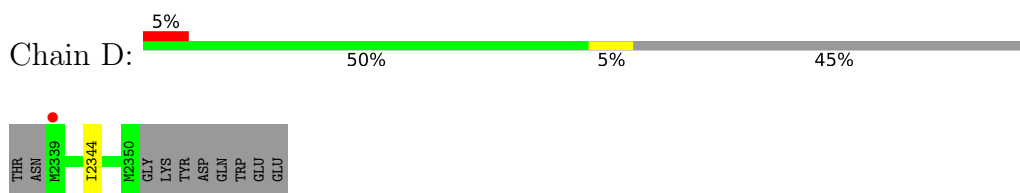
- Molecule 1: Peroxisome proliferator-activated receptor gamma



- Molecule 2: Nuclear receptor corepressor 2



- Molecule 2: Nuclear receptor corepressor 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.14Å 59.70Å 92.94Å 90.00° 105.99° 90.00°	Depositor
Resolution (Å)	41.88 – 2.50 41.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (41.88-2.50) 97.5 (41.88-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.234 , 0.285 0.234 , 0.285	Depositor DCC
$R_{free}$ test set	1137 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtrriage
Anisotropy	0.267	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A8R

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	0.24	0/2096	0.38	0/2821
1	B	0.24	0/2065	0.40	0/2782
2	C	0.22	0/111	0.39	0/144
2	D	0.23	0/90	0.39	0/117
All	All	0.24	0/4362	0.39	0/5864

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 [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	2063	0	2120	17	0
1	B	2033	0	2086	22	0
2	C	112	0	128	3	0
2	D	91	0	106	1	0
3	A	40	0	0	0	0
3	B	40	0	0	0	0
4	A	106	0	0	3	0
4	B	76	0	0	1	0
4	C	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	4	0	0	0	0
All	All	4570	0	4440	40	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 (40) 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:239:GLY:O	1:B:244:LYS:NZ	2.23	0.71
1:B:312:ASN:ND2	4:B:602:HOH:O	2.28	0.65
1:A:277:VAL:HG12	1:A:280:ARG:HH22	1.68	0.57
1:B:228:LEU:HD22	1:B:343:GLU:HA	1.88	0.55
1:B:241:THR:O	1:B:244:LYS:HD3	2.07	0.55
1:B:288:ARG:NH1	1:B:291:GLU:OE1	2.40	0.55
1:A:440:THR:HG21	1:B:443:ARG:HD2	1.89	0.54
1:B:214:LEU:HD21	1:B:413:LEU:HD23	1.90	0.54
1:A:250:TYR:O	4:A:601:HOH:O	2.18	0.53
1:B:301:LYS:HE2	2:C:2349:LEU:HA	1.89	0.53
1:B:247:PHE:HB3	1:B:264:PHE:HZ	1.74	0.53
1:B:350:ARG:NH2	1:B:365:GLU:OE2	2.37	0.50
1:A:267:ILE:HG22	1:A:271:GLN:HG3	1.94	0.50
1:B:454:GLN:HG2	1:B:457:LYS:HD2	1.94	0.50
1:A:380:ASP:OD2	1:A:424:ASN:ND2	2.41	0.50
2:C:2338:ASN:HB2	2:C:2341:LEU:HB2	1.97	0.47
1:A:234:ARG:NH2	4:A:617:HOH:O	2.44	0.47
1:A:353:LEU:HD13	1:A:364:MET:HG2	1.97	0.45
1:A:241:THR:OG1	1:A:243:ASP:OD1	2.27	0.45
1:B:445:ILE:O	1:B:449:HIS:N	2.49	0.45
1:B:275:LYS:O	1:B:280:ARG:NH1	2.50	0.45
1:B:229:THR:HG23	1:B:232:LYS:H	1.81	0.45
2:C:2347:LYS:NZ	4:C:2401:HOH:O	2.17	0.45
1:B:390:VAL:O	1:B:410:GLN:NE2	2.45	0.44
1:B:275:LYS:HA	1:B:275:LYS:HD2	1.77	0.43
1:B:357:ARG:HH22	1:B:360:PHE:HE2	1.66	0.43
1:A:290:VAL:HG13	2:D:2344:ILE:HD13	1.99	0.43
1:B:447:THR:HA	1:B:450:VAL:HG12	2.00	0.43
1:A:456:ILE:O	1:A:460:GLU:HB2	2.18	0.43
1:B:452:LEU:C	1:B:454:GLN:H	2.22	0.43
1:B:448:GLU:HA	1:B:451:GLN:HG2	2.01	0.42
1:A:260:ASP:N	1:A:260:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG12	1:A:280:ARG:NH2	2.34	0.42
1:A:221:SER:HA	1:A:224:LYS:HG2	2.02	0.41
1:A:230:LYS:O	1:A:234:ARG:HG2	2.21	0.41
1:A:422:LYS:NZ	4:A:615:HOH:O	2.44	0.41
1:A:243:ASP:O	1:A:244:LYS:HG2	2.21	0.41
1:B:456:ILE:HB	1:B:460:GLU:HG2	2.02	0.41
1:A:219:TYR:O	1:A:223:ILE:HG12	2.21	0.40
1:B:363:PHE:CD2	1:B:364:MET:HG2	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	255/290 (88%)	243 (95%)	12 (5%)	0	100	100
1	B	252/290 (87%)	239 (95%)	13 (5%)	0	100	100
2	C	13/22 (59%)	13 (100%)	0	0	100	100
2	D	10/22 (46%)	9 (90%)	1 (10%)	0	100	100
All	All	530/624 (85%)	504 (95%)	26 (5%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	229/262 (87%)	222 (97%)	7 (3%)	40	67
1	B	226/262 (86%)	222 (98%)	4 (2%)	59	81
2	C	11/18 (61%)	9 (82%)	2 (18%)	1	3
2	D	9/18 (50%)	9 (100%)	0	100	100
All	All	475/560 (85%)	462 (97%)	13 (3%)	44	71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	272	GLU
1	A	275	LYS
1	A	288	ARG
1	A	357	ARG
1	A	358	LYS
1	A	427	GLU
1	B	216	LYS
1	B	234	ARG
1	B	322	VAL
1	B	456	ILE
2	C	2339	MET
2	C	2341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides 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
3	A8R	A	501	-	41,43,43	1.87	8 (19%)	55,64,64	1.34	5 (9%)
3	A8R	B	501	-	41,43,43	1.88	9 (21%)	55,64,64	1.15	3 (5%)

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	A8R	A	501	-	-	9/30/30/30	0/4/4/4
3	A8R	B	501	-	-	2/30/30/30	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	A8R	C24-N26	7.08	1.49	1.34
3	A	501	A8R	C24-N26	7.00	1.49	1.34
3	A	501	A8R	O19-C17	4.14	1.44	1.37
3	B	501	A8R	O19-C17	4.01	1.44	1.37
3	A	501	A8R	O25-C24	-3.66	1.15	1.23
3	B	501	A8R	O25-C24	-3.66	1.15	1.23
3	A	501	A8R	C09-C05	2.93	1.43	1.40
3	B	501	A8R	C09-C05	2.77	1.43	1.40
3	B	501	A8R	C16-CL40	2.55	1.79	1.73
3	B	501	A8R	C11-C08	2.47	1.54	1.49
3	A	501	A8R	C27-N26	-2.45	1.42	1.47
3	A	501	A8R	C11-C08	2.45	1.54	1.49
3	A	501	A8R	C16-CL40	2.43	1.79	1.73
3	A	501	A8R	C08-N07	-2.37	1.34	1.39
3	B	501	A8R	C08-N07	-2.32	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	A8R	C27-N26	-2.28	1.42	1.47
3	B	501	A8R	O19-C20	-2.19	1.39	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	A8R	O19-C17-C16	5.23	120.73	116.13
3	B	501	A8R	O19-C17-C16	3.47	119.18	116.13
3	B	501	A8R	C09-C08-N07	3.41	108.83	106.66
3	A	501	A8R	C09-C08-N07	3.14	108.66	106.66
3	A	501	A8R	C13-C12-N07	-3.03	107.92	112.63
3	A	501	A8R	C11-C08-N07	2.55	125.90	122.69
3	B	501	A8R	C11-C08-N07	2.51	125.85	122.69
3	A	501	A8R	O19-C20-C39	2.16	110.83	106.82

There are no chirality outliers.

All (11) torsion outliers are listed below:

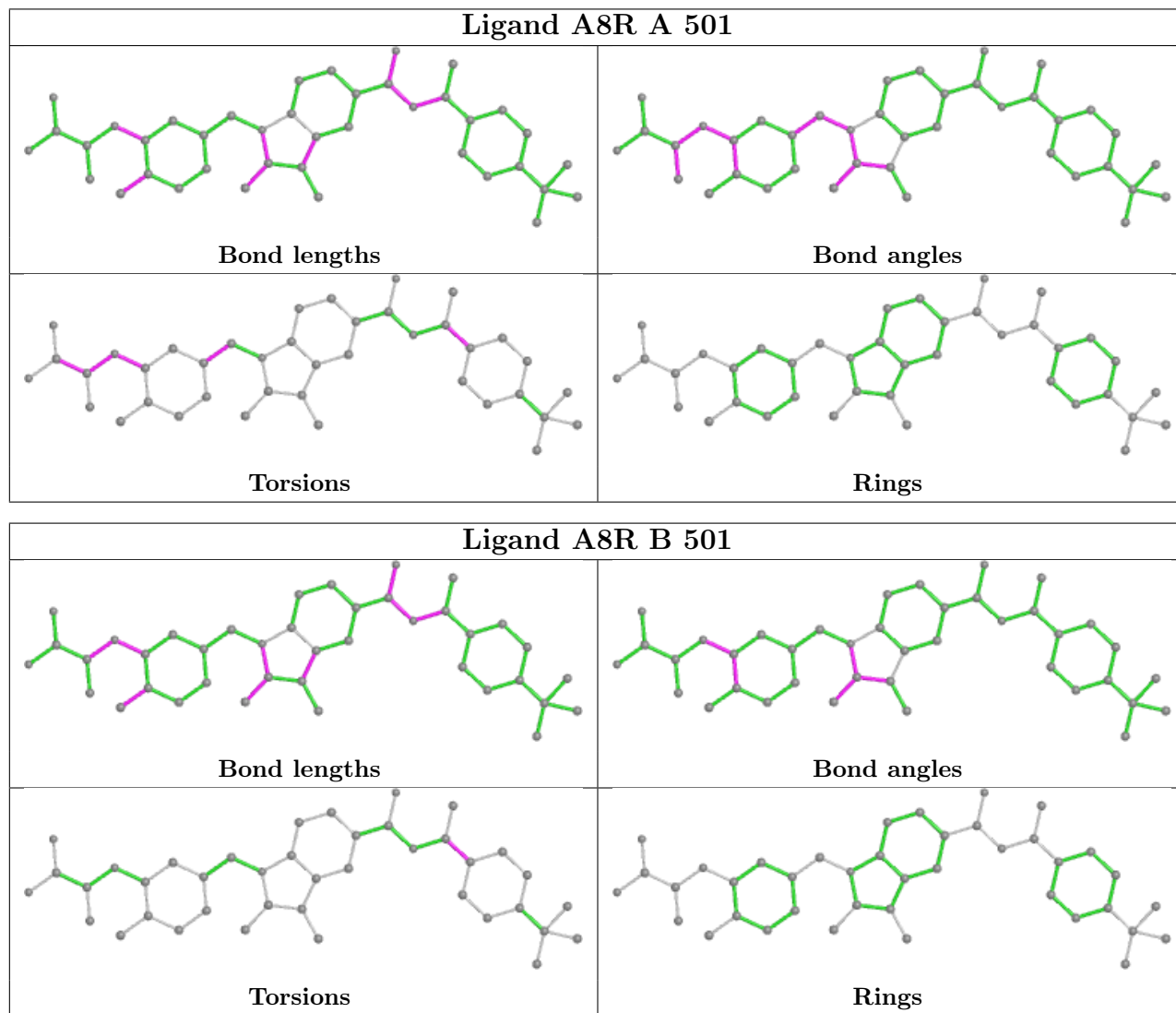
Mol	Chain	Res	Type	Atoms
3	A	501	A8R	C16-C17-O19-C20
3	A	501	A8R	C39-C20-C21-O23
3	A	501	A8R	C39-C20-O19-C17
3	A	501	A8R	C39-C20-C21-O22
3	A	501	A8R	C18-C17-O19-C20
3	A	501	A8R	C34-C27-C28-C33
3	B	501	A8R	C34-C27-C28-C29
3	A	501	A8R	N07-C12-C13-C18
3	A	501	A8R	N07-C12-C13-C14
3	A	501	A8R	C34-C27-C28-C29
3	B	501	A8R	C34-C27-C28-C33

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 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	259/290 (89%)	0.37	19 (7%) 15 15	34, 54, 120, 178	0
1	B	256/290 (88%)	0.31	17 (6%) 18 19	34, 58, 118, 205	0
2	C	15/22 (68%)	1.51	5 (33%) 0 0	66, 81, 143, 182	0
2	D	12/22 (54%)	0.73	1 (8%) 11 11	55, 78, 121, 123	0
All	All	542/624 (86%)	0.38	42 (7%) 13 13	34, 57, 121, 205	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	2352	LYS	8.0
1	B	459	THR	6.2
1	A	274	SER	4.8
1	A	245	SER	4.7
1	B	202	MET	4.6
2	C	2347	LYS	4.6
1	A	272	GLU	4.4
1	B	456	ILE	3.9
1	A	267	ILE	3.8
1	A	279	ILE	3.8
1	B	264	PHE	3.8
1	A	357	ARG	3.7
1	B	274	SER	3.6
1	B	452	LEU	3.5
1	A	358	LYS	3.4
1	A	263	LYS	3.3
2	D	2339	MET	3.3
1	B	450	VAL	3.3
1	A	262	ILE	3.1
2	C	2339	MET	3.1
1	A	459	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	453	LEU	3.0
1	A	273	GLN	2.8
1	A	244	LYS	2.7
1	B	266	HIS	2.7
1	B	356	LEU	2.6
2	C	2351	GLY	2.6
1	B	311	LEU	2.5
1	B	244	LYS	2.5
1	A	439	MET	2.5
1	B	460	GLU	2.5
1	A	275	LYS	2.4
1	B	457	LYS	2.4
1	B	454	GLN	2.3
1	A	429	SER	2.2
1	A	266	HIS	2.1
1	A	260	ASP	2.1
1	A	451	GLN	2.1
1	A	308	ASN	2.1
1	B	358	LYS	2.1
2	C	2348	ALA	2.0
1	B	277	VAL	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 monosaccharides in this entry.

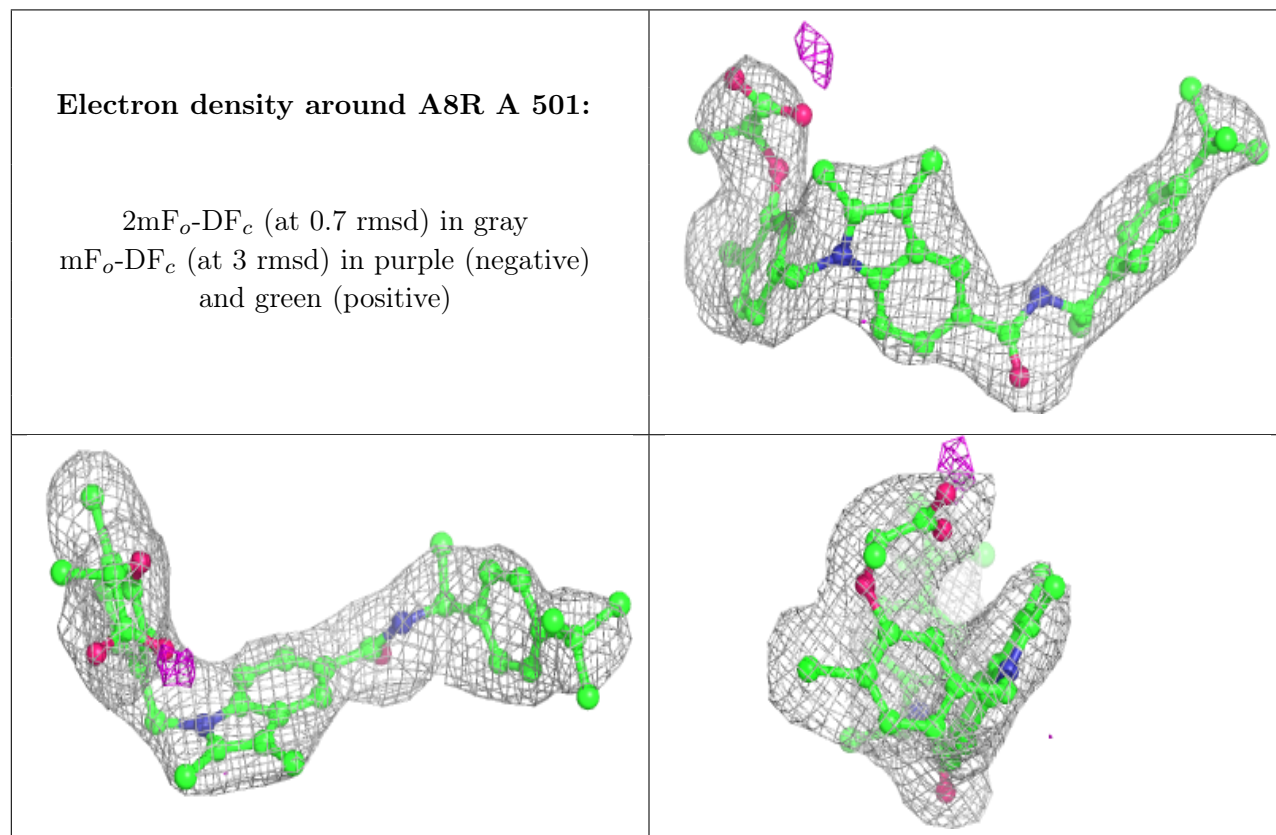
## 6.4 Ligands [i](#)

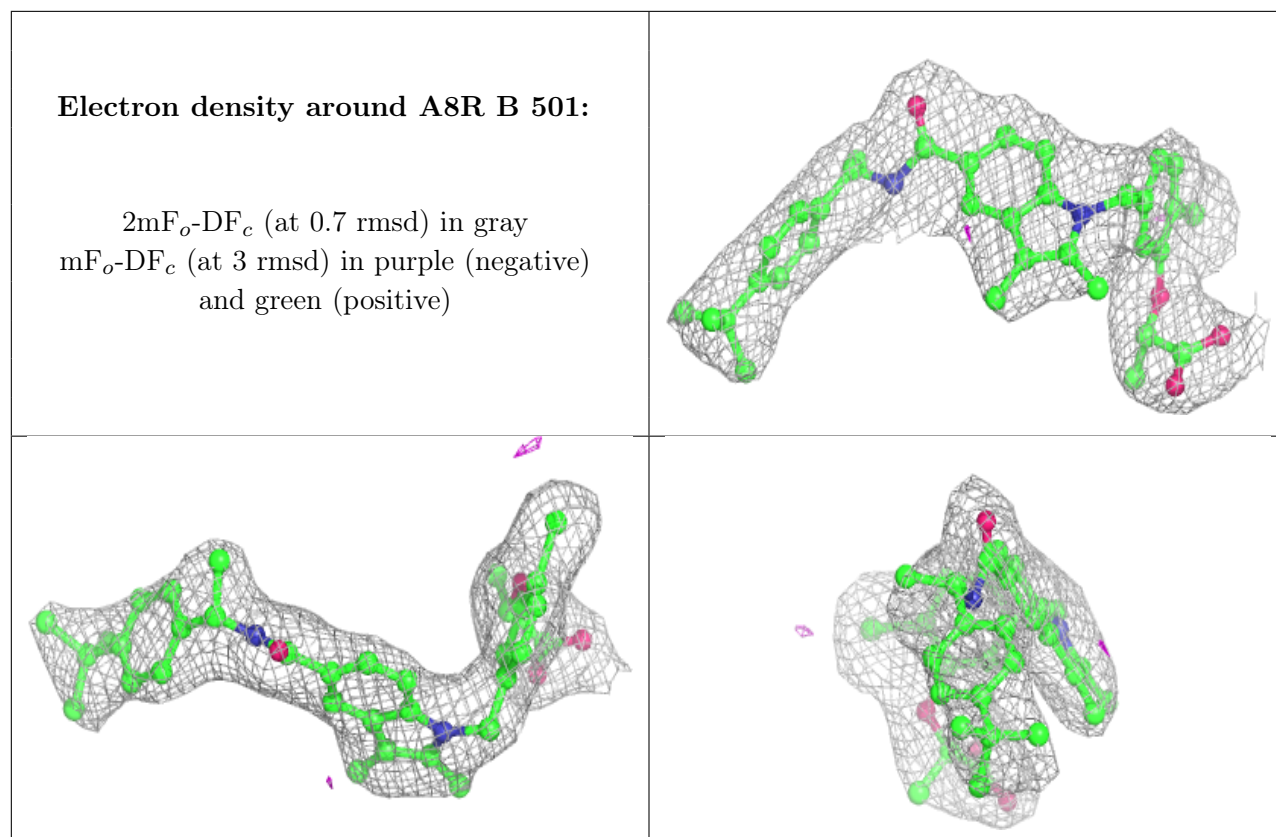
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	A8R	A	501	40/40	0.92	0.20	62,68,75,77	0
3	A8R	B	501	40/40	0.93	0.18	51,59,66,68	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.