



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:16 pm BST

PDB ID : 2Q6R  
Title : Crystal structure of PPAR gamma complexed with partial agonist SF147  
Authors : Bruning, J.B.; Nettles, K.W.  
Deposited on : 2007-06-01  
Resolution : 2.41 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.

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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 : 2.11  
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

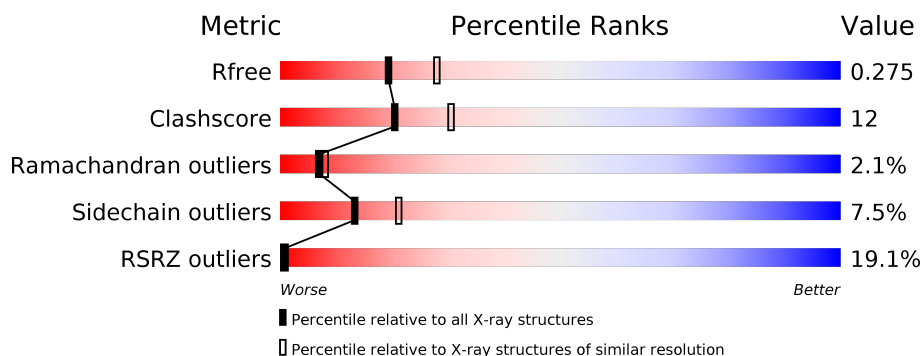
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	274	<div> <div>18%</div> <div>67%</div> <div>17%</div> <div>••</div> <div>14%</div> </div>
1	B	274	<div> <div>16%</div> <div>69%</div> <div>20%</div> <div>••</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF2	A	5001	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4069 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.

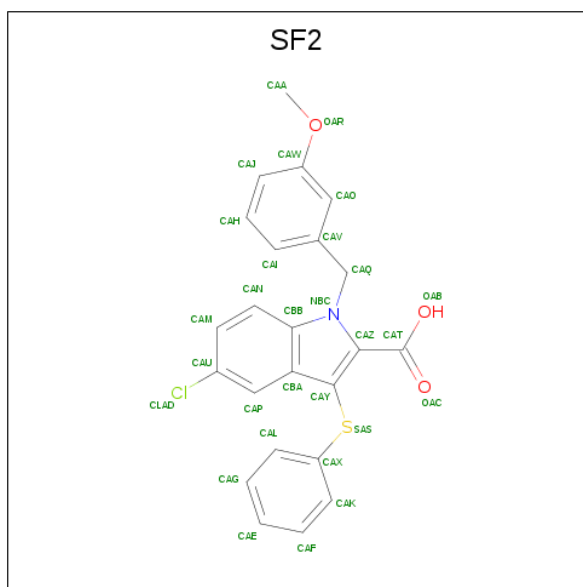
- Molecule 1 is a protein called Peroxisome Proliferator-Activated Receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1839	1182	295	353	9			
1	B	258	Total	C	N	O	S	0	0	0
			2048	1324	336	379	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	SER	-	EXPRESSION TAG	UNP P37231
B	204	SER	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is 5-CHLORO-1-(3-METHOXYBENZYL)-3-(PHENYLTHIO)-1H-INDOLE-2-CARBOXYLIC ACID (three-letter code: SF2) (formula: C<sub>23</sub>H<sub>18</sub>ClNO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			29	23	1	1	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	S	0	0
			29	23	1	1	3	1		

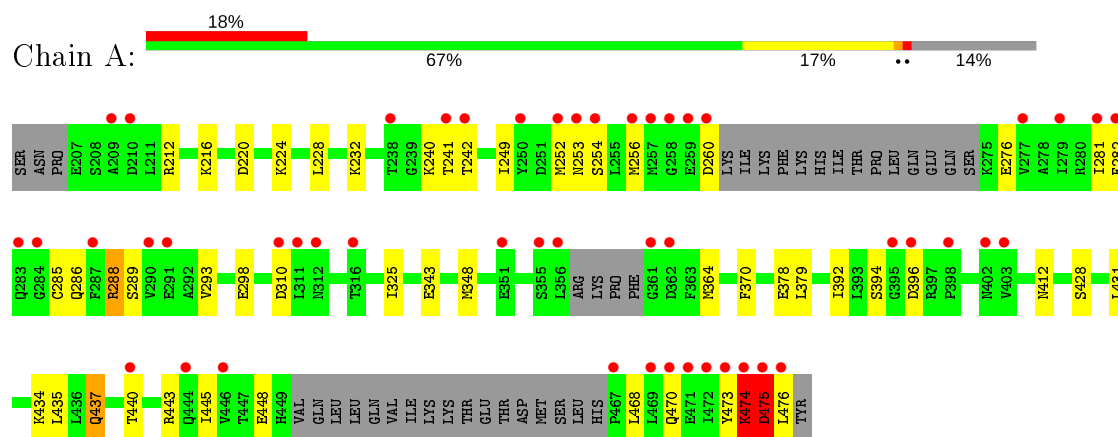
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	68	Total	O	0	0
			68	68		

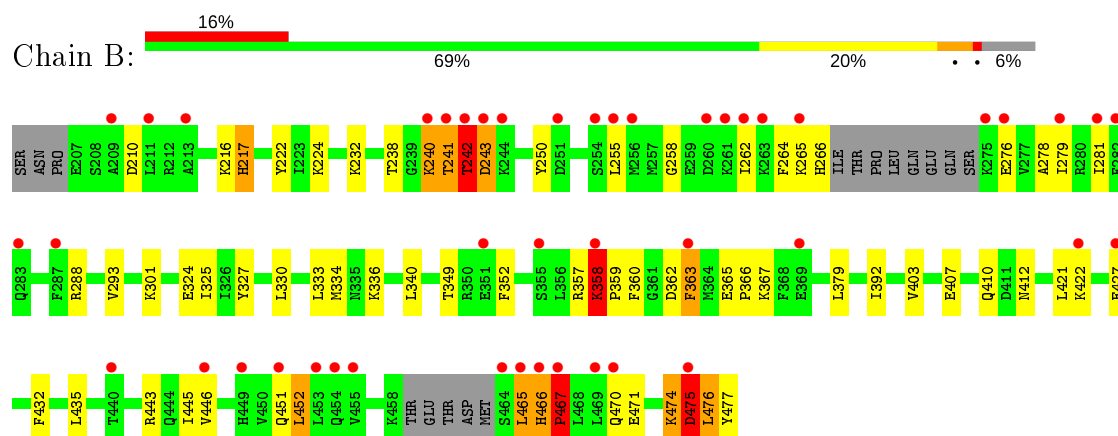
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	90.80 Å   62.26 Å   118.07 Å 90.00°   101.12°   90.00°	Depositor
Resolution (Å)	10.00 – 2.41 10.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	90.9 (10.00-2.41) 90.9 (10.00-2.41)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.77 (at 2.41 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.269   ,   0.284 0.264   ,   0.275	Depositor DCC
$R_{free}$ test set	1146 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.1	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF2

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	0.42	0/1865	0.84	4/2516 (0.2%)
1	B	0.47	1/2081 (0.0%)	0.58	2/2802 (0.1%)
All	All	0.45	1/3946 (0.0%)	0.72	6/5318 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	1	7
All	All	2	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	LYS	CE-NZ	6.91	1.66	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ASP	N-CA-C	21.73	169.66	111.00
1	A	475	ASP	CB-CA-C	-18.43	73.55	110.40
1	A	475	ASP	C-N-CA	12.65	153.32	121.70
1	B	243	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	475	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	475	ASP	CB-CG-OD2	5.09	122.88	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	475	ASP	CA
1	B	466	HIS	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	LYS	Peptide
1	A	475	ASP	Peptide
1	B	240	LYS	Peptide
1	B	242	THR	Peptide
1	B	243	ASP	Peptide
1	B	465	LEU	Peptide
1	B	467	PRO	Peptide
1	B	475	ASP	Peptide
1	B	476	LEU	Peptide

## 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	1839	0	1842	41	0
1	B	2048	0	2088	57	0
2	A	29	0	17	10	0
2	B	29	0	17	2	0
3	A	56	0	0	7	0
3	B	68	0	0	2	0
All	All	4069	0	3964	98	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 12.

All (98) 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:474:LYS:HE2	1:A:474:LYS:CA	1.53	1.31
1:A:474:LYS:HA	1:A:474:LYS:CE	1.55	1.28
1:B:358:LYS:HB3	1:B:359:PRO:CD	1.72	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LYS:O	1:B:241:THR:HG23	1.56	1.04
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.09	1.04
1:A:476:LEU:HD22	3:A:92:HOH:O	1.56	1.03
1:B:293:VAL:HG21	1:B:476:LEU:CB	1.89	1.01
1:A:394:SER:HB3	3:A:105:HOH:O	1.68	0.93
1:B:363:PHE:HB2	1:B:452:LEU:CD2	2.08	0.84
1:B:242:THR:O	1:B:242:THR:HG22	1.76	0.83
1:A:474:LYS:O	1:A:475:ASP:HB2	1.76	0.82
1:B:358:LYS:CB	1:B:359:PRO:HD3	2.03	0.82
1:B:217:HIS:O	1:B:217:HIS:CD2	2.33	0.82
1:A:474:LYS:CA	1:A:474:LYS:CE	2.30	0.82
1:B:327:TYR:HE2	1:B:367:LYS:HE2	1.44	0.79
2:A:5001:SF2:HAP	3:A:113:HOH:O	1.83	0.78
1:B:217:HIS:CD2	1:B:217:HIS:C	2.57	0.77
1:B:358:LYS:CB	1:B:359:PRO:CD	2.57	0.77
1:B:362:ASP:O	1:B:363:PHE:HB3	1.81	0.77
1:B:466:HIS:H	1:B:470:GLN:HG3	1.51	0.75
1:A:288:ARG:HG3	2:A:5001:SF2:CAT	2.15	0.75
1:B:240:LYS:O	1:B:241:THR:CG2	2.34	0.74
1:B:258:GLY:O	1:B:262:ILE:HB	1.89	0.73
1:A:474:LYS:N	1:A:474:LYS:HE2	2.03	0.72
1:A:476:LEU:CD2	3:A:92:HOH:O	2.23	0.72
1:A:474:LYS:HA	1:A:474:LYS:HE2	0.75	0.70
1:B:363:PHE:HB2	1:B:452:LEU:HD22	1.71	0.70
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.73	0.70
1:B:327:TYR:CE2	1:B:367:LYS:HE2	2.28	0.69
1:B:363:PHE:HB2	1:B:452:LEU:HD21	1.74	0.68
1:A:364:MET:HE2	2:A:5001:SF2:HAM	1.75	0.68
1:B:327:TYR:HE2	1:B:367:LYS:CE	2.09	0.65
1:B:301:LYS:O	3:B:65:HOH:O	2.13	0.65
1:B:238:THR:OG1	1:B:240:LYS:HB2	1.96	0.65
1:A:428:SER:HB3	1:A:431:LEU:HB2	1.79	0.65
1:B:242:THR:O	1:B:242:THR:CG2	2.46	0.63
1:A:281:ILE:HG23	3:A:113:HOH:O	1.97	0.63
1:B:330:LEU:HD23	1:B:367:LYS:HD3	1.81	0.63
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.81	0.61
1:B:470:GLN:O	1:B:474:LYS:HB3	2.01	0.61
1:B:474:LYS:HG2	1:B:475:ASP:N	2.16	0.60
1:A:364:MET:CE	2:A:5001:SF2:HAM	2.31	0.60
1:A:474:LYS:O	1:A:475:ASP:CB	2.47	0.59
1:A:370:PHE:CB	1:A:445:ILE:HD11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:O	1:B:334:MET:HG3	2.04	0.58
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.33	0.58
1:B:363:PHE:CD1	1:B:363:PHE:O	2.57	0.56
1:A:440:THR:HG21	1:B:443:ARG:HD2	1.88	0.55
1:B:324:GLU:HG3	1:B:446:VAL:HG21	1.89	0.55
1:B:333:LEU:HB3	1:B:340:LEU:HB2	1.87	0.55
1:B:240:LYS:C	1:B:241:THR:HG23	2.26	0.54
1:B:362:ASP:O	1:B:363:PHE:CB	2.53	0.53
2:A:5001:SF2:HAI	2:A:5001:SF2:CBB	2.38	0.53
1:B:217:HIS:O	1:B:217:HIS:CG	2.61	0.53
1:B:293:VAL:CG2	1:B:476:LEU:CB	2.77	0.52
1:A:212:ARG:HD2	3:A:73:HOH:O	2.11	0.51
1:A:470:GLN:O	1:A:474:LYS:HE3	2.11	0.51
1:A:348:MET:HE1	2:A:5001:SF2:HAF	1.92	0.51
2:B:7001:SF2:CBB	2:B:7001:SF2:HAI	2.41	0.51
1:B:476:LEU:O	1:B:477:TYR:CB	2.59	0.50
1:A:348:MET:CE	2:A:5001:SF2:HAF	2.41	0.50
1:B:403:VAL:HG12	1:B:407:GLU:HG3	1.92	0.50
1:A:282:PHE:O	1:A:286:GLN:HB2	2.11	0.50
1:A:253:ASN:HA	1:A:256:MET:HB3	1.95	0.49
1:B:465:LEU:O	1:B:466:HIS:CB	2.60	0.49
1:B:471:GLU:O	1:B:474:LYS:NZ	2.46	0.49
1:B:240:LYS:O	1:B:241:THR:OG1	2.31	0.48
1:A:288:ARG:CG	2:A:5001:SF2:CAT	2.89	0.48
1:A:228:LEU:HD12	1:A:232:LYS:HD2	1.95	0.48
1:A:437:GLN:OE1	1:B:410:GLN:NE2	2.46	0.47
1:B:379:LEU:HD11	1:B:435:LEU:HD13	1.97	0.47
1:A:285:CYS:HB2	2:A:5001:SF2:CAP	2.45	0.47
1:B:466:HIS:HA	1:B:467:PRO:HA	1.59	0.47
1:B:365:GLU:N	1:B:366:PRO:HD2	2.30	0.47
1:A:474:LYS:N	1:A:474:LYS:CE	2.71	0.47
1:B:232:LYS:HB2	1:B:232:LYS:HE3	1.69	0.46
1:A:288:ARG:HG3	2:A:5001:SF2:OAB	2.15	0.46
1:A:289:SER:O	1:A:293:VAL:HG23	2.16	0.46
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.97	0.46
1:B:240:LYS:O	1:B:241:THR:CB	2.63	0.45
1:B:255:LEU:HD22	1:B:352:PHE:CZ	2.51	0.45
1:B:222:TYR:HD1	3:B:118:HOH:O	1.99	0.45
1:B:279:ILE:HD12	1:B:360:PHE:HZ	1.80	0.45
1:A:440:THR:CG2	1:B:443:ARG:HD2	2.45	0.45
1:B:278:ALA:HA	1:B:281:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:HD12	1:B:432:PHE:HA	1.99	0.43
1:B:276:GLU:O	1:B:279:ILE:HG22	2.19	0.43
1:B:288:ARG:HG2	2:B:7001:SF2:CAT	2.49	0.42
1:A:249:ILE:HA	1:A:254:SER:HB3	2.01	0.42
1:A:288:ARG:HA	1:A:288:ARG:HD2	1.73	0.42
1:A:228:LEU:HB2	1:A:343:GLU:HG3	2.02	0.42
1:B:250:TYR:HA	1:B:349:THR:OG1	2.20	0.41
1:A:473:TYR:O	1:A:475:ASP:N	2.54	0.41
1:B:241:THR:HB	1:B:242:THR:H	1.73	0.41
1:B:325:ILE:HD11	1:B:392:ILE:HG13	2.01	0.41
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.51	0.41
1:A:298:GLU:HG3	3:A:39:HOH:O	2.22	0.40
1:A:220:ASP:O	1:A:224:LYS:HD2	2.21	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	227/274 (83%)	209 (92%)	14 (6%)	4 (2%)	8	10
1	B	252/274 (92%)	234 (93%)	12 (5%)	6 (2%)	6	6
All	All	479/548 (87%)	443 (92%)	26 (5%)	10 (2%)	7	8

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	THR
1	B	357	ARG
1	B	358	LYS
1	B	466	HIS
1	A	242	THR

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Mol	Chain	Res	Type
1	B	264	PHE
1	A	474	LYS
1	A	276	GLU
1	B	467	PRO
1	A	310	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	201/247 (81%)	187 (93%)	14 (7%)	15	24
1	B	224/247 (91%)	206 (92%)	18 (8%)	12	18
All	All	425/494 (86%)	393 (92%)	32 (8%)	13	21

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	241	THR
1	A	252	MET
1	A	260	ASP
1	A	288	ARG
1	A	378	GLU
1	A	396	ASP
1	A	412	ASN
1	A	434	LYS
1	A	437	GLN
1	A	443	ARG
1	A	448	GLU
1	A	468	LEU
1	A	474	LYS
1	B	210	ASP
1	B	216	LYS
1	B	217	HIS
1	B	224	LYS

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Mol	Chain	Res	Type
1	B	242	THR
1	B	265	LYS
1	B	266	HIS
1	B	336	LYS
1	B	358	LYS
1	B	363	PHE
1	B	412	ASN
1	B	422	LYS
1	B	427	GLU
1	B	445	ILE
1	B	451	GLN
1	B	452	LEU
1	B	474	LYS
1	B	475	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	GLN
1	B	217	HIS
1	B	410	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	SF2	A	5001	-	25,32,32	0.94	1 (4%)	32,45,45	1.61	3 (9%)
2	SF2	B	7001	-	25,32,32	0.92	0	32,45,45	1.41	4 (12%)

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	SF2	A	5001	-	-	4/10/14/14	0/4/4/4
2	SF2	B	7001	-	-	4/10/14/14	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	SF2	CAQ-CAV	2.26	1.56	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	SF2	CAX-SAS-CAY	6.60	117.81	101.93
2	B	7001	SF2	CAX-SAS-CAY	4.66	113.13	101.93
2	B	7001	SF2	CAV-CAQ-NBC	-3.77	106.77	112.63
2	A	5001	SF2	CAV-CAQ-NBC	-3.55	107.11	112.63
2	B	7001	SF2	CAY-CBA-CBB	-2.65	107.01	114.39
2	A	5001	SF2	CAY-CBA-CBB	-2.59	107.18	114.39
2	B	7001	SF2	CAA-OAR-CAW	-2.27	112.57	117.51

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5001	SF2	CAO-CAW-OAR-CAA

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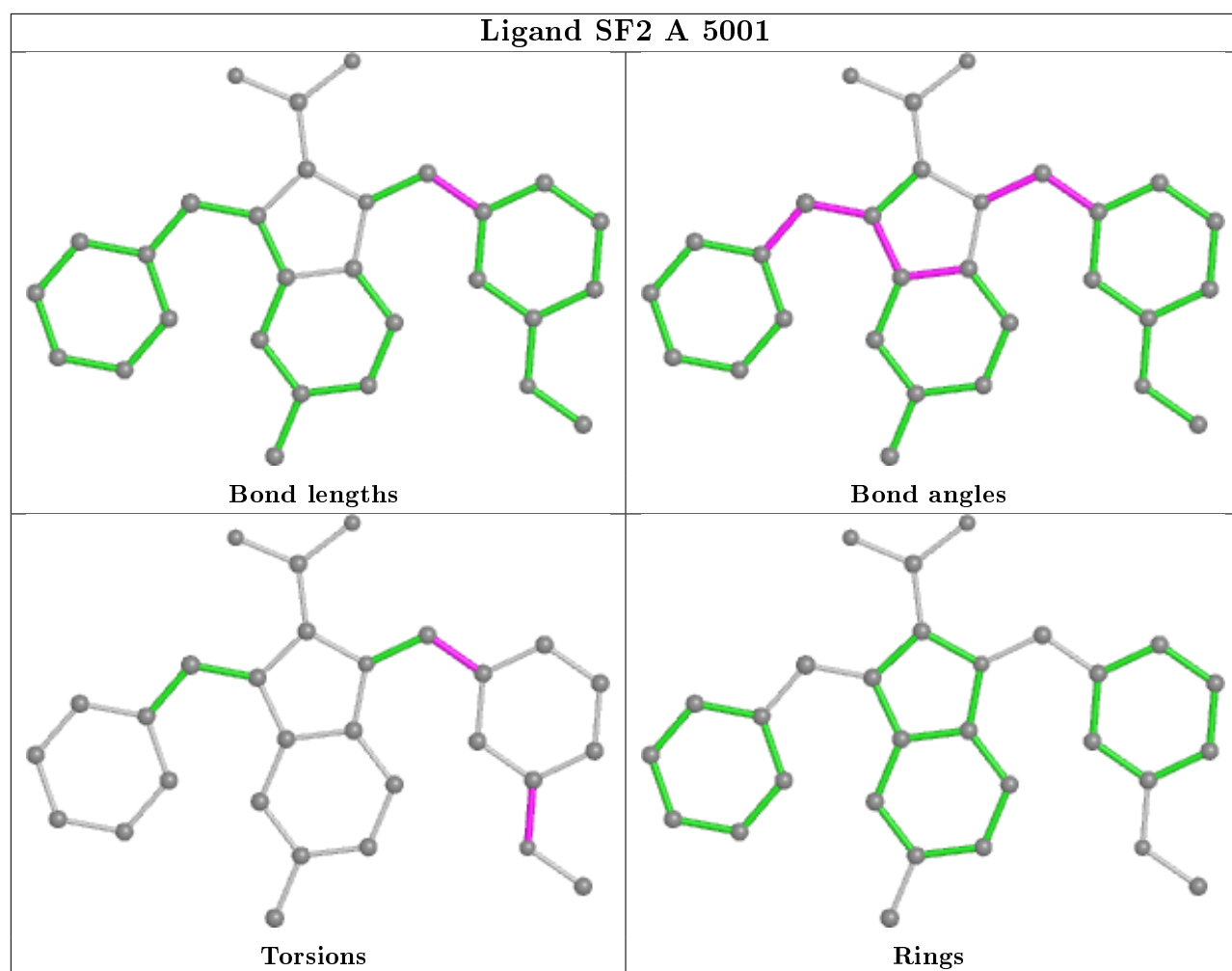
Mol	Chain	Res	Type	Atoms
2	A	5001	SF2	CAJ-CAW-OAR-CAA
2	B	7001	SF2	CAO-CAW-OAR-CAA
2	B	7001	SF2	CAJ-CAW-OAR-CAA
2	B	7001	SF2	NBC-CAQ-CAV-CAI
2	B	7001	SF2	NBC-CAQ-CAV-CAO
2	A	5001	SF2	NBC-CAQ-CAV-CAI
2	A	5001	SF2	NBC-CAQ-CAV-CAO

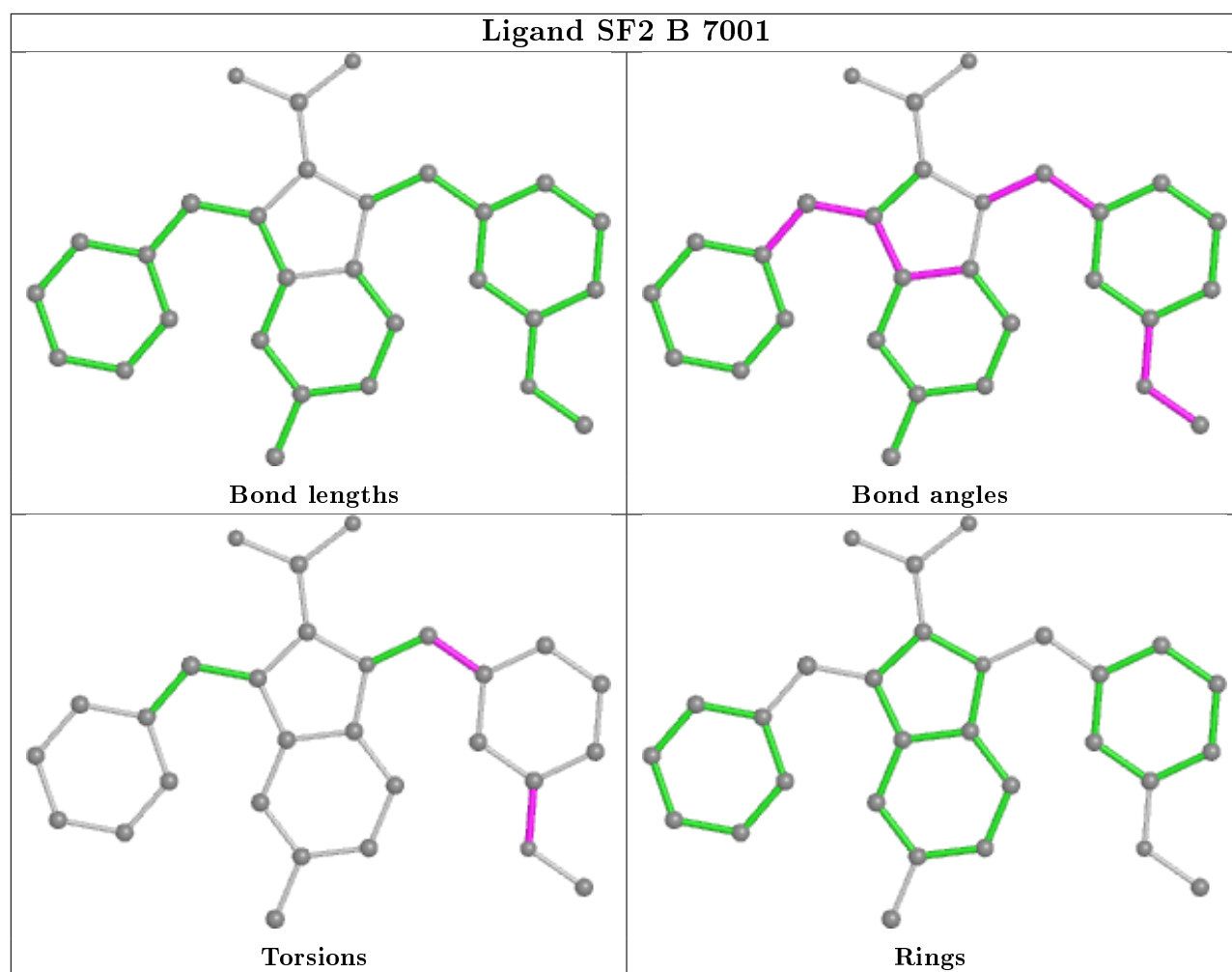
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	SF2	10	0
2	B	7001	SF2	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 [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, 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	235/274 (85%)	1.06	49 (20%) <b>1</b> <b>0</b>	47, 90, 173, 225	5 (2%)
1	B	258/274 (94%)	0.80	45 (17%) <b>1</b> <b>1</b>	39, 71, 137, 156	0
All	All	493/548 (89%)	0.92	94 (19%) <b>1</b> <b>0</b>	39, 82, 155, 225	5 (1%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	THR	13.0
1	B	243	ASP	10.0
1	A	470	GLN	7.9
1	A	260	ASP	6.7
1	B	454	GLN	6.2
1	A	475	ASP	6.0
1	A	471	GLU	5.6
1	B	256	MET	5.5
1	B	470	GLN	5.5
1	B	241	THR	5.4
1	A	259	GLU	4.7
1	A	282	PHE	4.5
1	B	469	LEU	4.4
1	A	440	THR	4.4
1	A	256	MET	4.3
1	A	469	LEU	4.2
1	B	287	PHE	4.2
1	B	451	GLN	4.2
1	A	398	PRO	4.1
1	B	260	ASP	4.0
1	A	257	MET	3.9
1	B	358	LYS	3.9
1	A	283	GLN	3.9
1	A	472	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	251	ASP	3.8
1	B	240	LYS	3.7
1	A	403	VAL	3.7
1	A	287	PHE	3.6
1	A	312	ASN	3.5
1	A	396	ASP	3.4
1	B	209	ALA	3.4
1	A	250	TYR	3.4
1	A	467	PRO	3.4
1	B	363	PHE	3.4
1	A	284	GLY	3.3
1	A	290	VAL	3.3
1	B	283	GLN	3.3
1	B	351	GLU	3.2
1	A	395	GLY	3.2
1	A	258	GLY	3.1
1	A	356	LEU	3.1
1	A	242	THR	3.1
1	B	453	LEU	3.0
1	B	465	LEU	3.0
1	A	311	LEU	2.9
1	B	467	PRO	2.9
1	B	466	HIS	2.9
1	A	473	TYR	2.9
1	A	444	GLN	2.9
1	A	210	ASP	2.8
1	A	474	LYS	2.8
1	A	351	GLU	2.8
1	B	440	THR	2.8
1	B	255	LEU	2.8
1	B	282	PHE	2.8
1	A	277	VAL	2.7
1	B	261	LYS	2.7
1	A	355	SER	2.7
1	B	475	ASP	2.7
1	B	276	GLU	2.7
1	A	279	ILE	2.7
1	B	262	ILE	2.7
1	A	253	ASN	2.7
1	B	275	LYS	2.7
1	B	449	HIS	2.7
1	A	310	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	254	SER	2.6
1	B	355	SER	2.6
1	A	209	ALA	2.6
1	A	316	THR	2.6
1	B	213	ALA	2.6
1	A	241	THR	2.5
1	A	476	LEU	2.5
1	B	244	LYS	2.5
1	B	211	LEU	2.5
1	A	362	ASP	2.4
1	B	265	LYS	2.4
1	A	238	THR	2.4
1	A	252	MET	2.4
1	B	281	ILE	2.4
1	B	464	SER	2.3
1	A	446	VAL	2.3
1	A	291	GLU	2.2
1	A	361	GLY	2.2
1	B	455	VAL	2.2
1	B	254	SER	2.2
1	B	263	LYS	2.1
1	B	369	GLU	2.1
1	B	422	LYS	2.1
1	A	402	ASN	2.1
1	B	427	GLU	2.0
1	B	279	ILE	2.0
1	B	446	VAL	2.0
1	A	281	ILE	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.

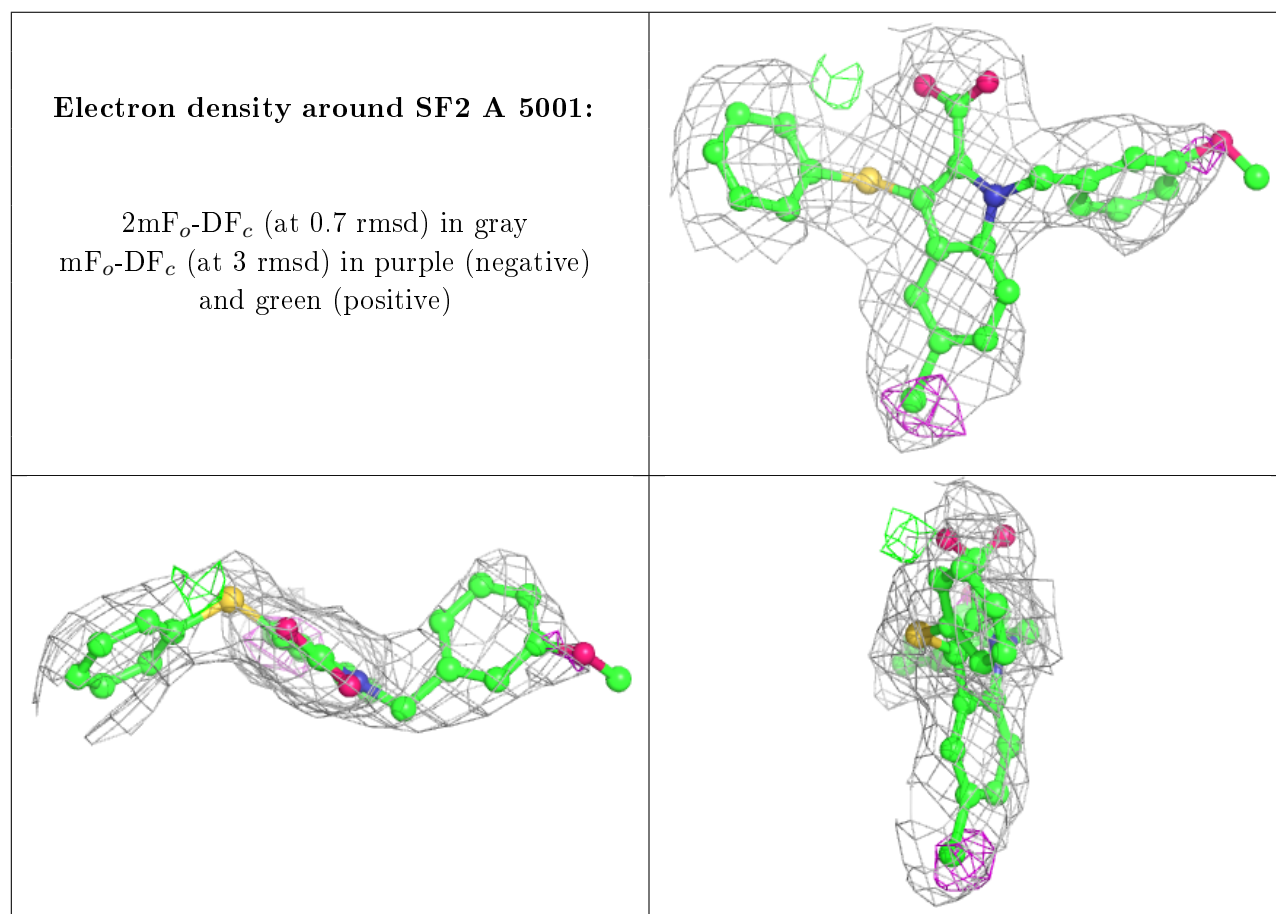
## 6.4 Ligands [i](#)

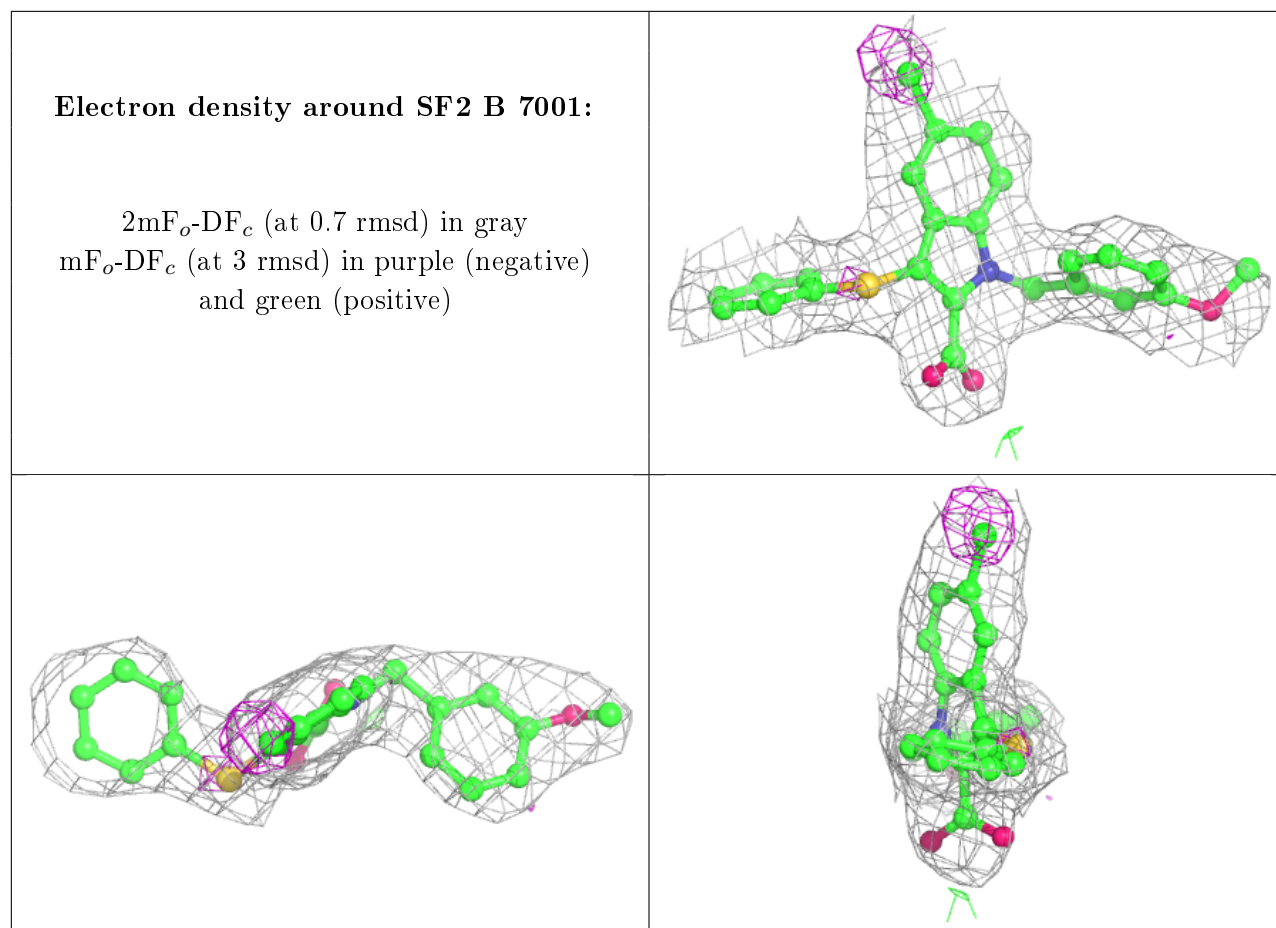
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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( $\text{\AA}^2$ )	Q<0.9
2	SF2	A	5001	29/29	0.81	0.22	60,77,85,87	0
2	SF2	B	7001	29/29	0.90	0.15	55,60,68,69	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 ⓘ

There are no such residues in this entry.