



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:38 am BST

PDB ID : 2G0H
Title : Structure-based drug design of a novel family of PPAR partial agonists: virtual screening, x-ray crystallography and in vitro/in vivo biological activities
Authors : Lu, I.L.; Peng, Y.H.; Huang, C.F.; Lin, Y.T.; Hsu, J.T.A.; Wu, S.Y.
Deposited on : 2006-02-13
Resolution : 2.30 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

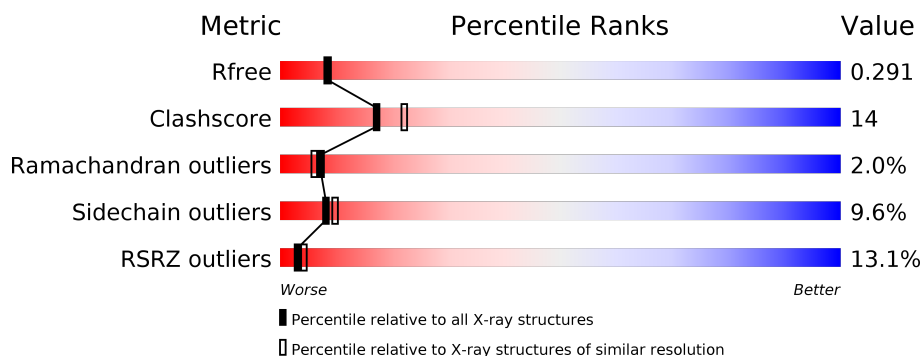
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	271	<div> <div>14%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>7%</div> </div> </div>
1	B	271	<div> <div>12%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>5%</div> </div> </div>

2 Entry composition [i](#)

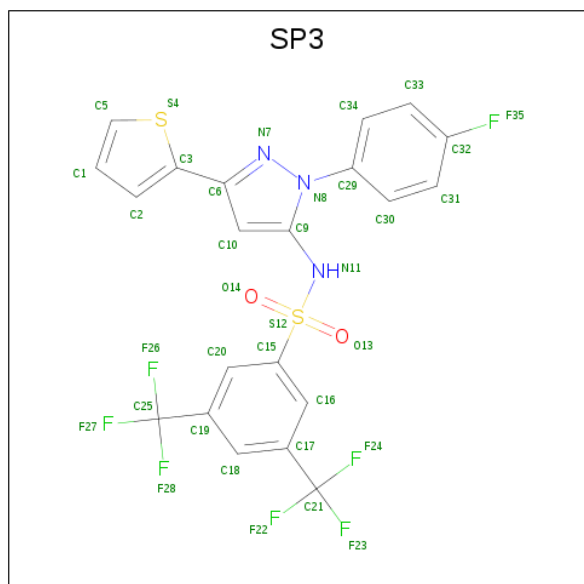
There are 3 unique types of molecules in this entry. The entry contains 4511 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	271	Total	C	N	O	S	0	0	0
			2177	1406	355	406	10			
1	B	271	Total	C	N	O	S	0	0	0
			2177	1406	355	406	10			

- Molecule 2 is N-[1-(4-FLUOROPHENYL)-3-(2-THIENYL)-1H-PYRAZOL-5-YL]-3,5-BIS(TRIFLUOROMETHYL)BENZENESULFONAMIDE (three-letter code: SP3) (formula: $C_{21}H_{12}F_7N_3O_2S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			35	21	7	3	2		
2	B	1	Total	C	F	N	O	0	0
			35	21	7	3	2		

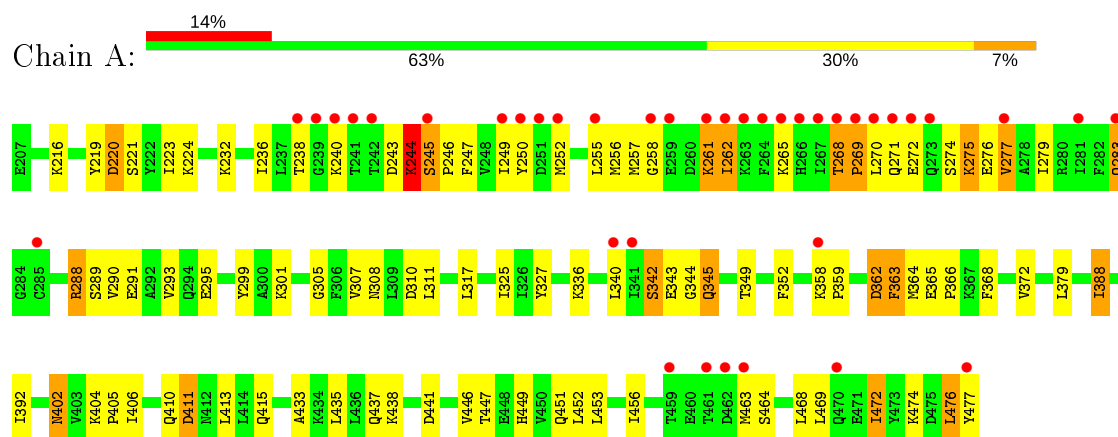
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total 23	O 23	0	0
3	B	64	Total 64	O 64	0	0

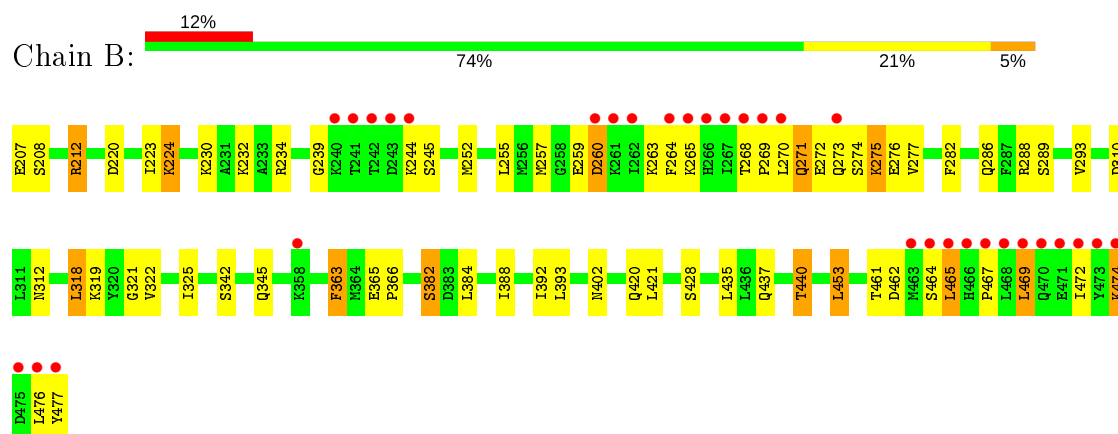
3 Residue-property plots [i](#)

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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.30Å 88.90Å 58.45Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.90 – 2.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 99.1 (19.90-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.238 , 0.293 0.237 , 0.291	Depositor DCC
R_{free} test set	1499 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.029 for h,-k,-l 0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4511	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: SP3

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	0.40	0/2215	0.83	1/2985 (0.0%)
1	B	0.48	0/2215	0.90	2/2985 (0.1%)
All	All	0.44	0/4430	0.87	3/5970 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ASP	N-CA-CB	7.37	123.87	110.60
1	B	212	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	207	GLU	OE1-CD-OE2	-5.18	117.08	123.30

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	2177	0	2241	67	0
1	B	2177	0	2241	56	0
2	A	35	0	12	4	0
2	B	35	0	12	4	0
3	A	23	0	0	2	0
3	B	64	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4511	0	4506	124	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 14.

All (124) 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:268:THR:HG22	1:B:268:THR:O	1.68	0.94
1:B:259:GLU:O	1:B:263:LYS:HB3	1.78	0.83
1:B:271:GLN:HA	1:B:271:GLN:HE21	1.44	0.80
1:B:275:LYS:HE3	1:B:276:GLU:H	1.44	0.80
1:B:271:GLN:HA	1:B:271:GLN:NE2	1.97	0.79
1:B:286:GLN:HE22	1:B:465:LEU:HB3	1.47	0.78
1:B:263:LYS:HE2	1:B:269:PRO:HG3	1.66	0.77
1:B:293:VAL:HG22	1:B:322:VAL:HG11	1.67	0.76
1:B:363:PHE:HZ	1:B:453:LEU:HD13	1.51	0.75
1:B:268:THR:O	1:B:268:THR:CG2	2.35	0.74
2:B:201:SP3:H11	2:B:201:SP3:H34	1.52	0.74
2:A:101:SP3:H11	2:A:101:SP3:H34	1.54	0.72
1:B:469:LEU:HA	1:B:472:ILE:HB	1.71	0.72
1:B:275:LYS:HD3	1:B:462:ASP:OD1	1.91	0.71
1:A:262:ILE:HG23	1:A:265:LYS:O	1.94	0.67
2:B:201:SP3:H11	2:B:201:SP3:C34	2.06	0.67
1:A:438:LYS:HE3	3:A:79:HOH:O	1.94	0.66
1:A:311:LEU:HD23	1:B:271:GLN:HG2	1.77	0.66
1:A:247:PHE:CZ	1:A:257:MET:HG2	2.31	0.65
1:A:301:LYS:NZ	1:B:467:PRO:HD2	2.11	0.65
1:A:364:MET:HE3	2:A:101:SP3:H10	1.81	0.62
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.63	0.62
1:A:247:PHE:HZ	1:A:257:MET:HG2	1.66	0.61
1:A:325:ILE:HG23	1:A:388:ILE:HG12	1.83	0.60
1:A:410:GLN:HA	1:A:413:LEU:HD12	1.82	0.60
2:A:101:SP3:H11	2:A:101:SP3:C34	2.14	0.59
1:A:255:LEU:CD2	1:A:277:VAL:HG13	2.33	0.59
1:A:275:LYS:HG3	1:A:283:GLN:NE2	2.18	0.58
1:A:238:THR:CG2	1:A:240:LYS:HG2	2.33	0.58
1:A:365:GLU:HB3	1:A:366:PRO:CD	2.33	0.58
1:B:220:ASP:O	1:B:224:LYS:HG3	2.05	0.56
1:A:255:LEU:HD21	1:A:277:VAL:HG13	1.86	0.56
2:B:201:SP3:N11	2:B:201:SP3:H34	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASP:OD2	1:B:269:PRO:HD2	2.06	0.56
1:B:472:ILE:O	1:B:472:ILE:HG22	2.06	0.56
1:A:220:ASP:O	1:A:224:LYS:HG3	2.06	0.56
1:A:252:MET:O	1:A:256:MET:HG3	2.06	0.55
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.89	0.54
1:B:293:VAL:HG22	1:B:322:VAL:CG1	2.38	0.53
1:A:238:THR:HG21	1:A:240:LYS:HE3	1.89	0.53
1:B:363:PHE:CZ	1:B:453:LEU:HD13	2.39	0.53
1:A:472:ILE:O	1:A:476:LEU:HD13	2.08	0.53
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.90	0.53
1:B:255:LEU:CD2	1:B:277:VAL:HG13	2.38	0.53
1:B:274:SER:O	1:B:275:LYS:HB3	2.09	0.52
1:A:327:TYR:HE2	1:A:446:VAL:HG22	1.74	0.52
1:B:271:GLN:CD	1:B:272:GLU:H	2.13	0.52
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.92	0.52
1:B:474:LYS:HB3	1:B:474:LYS:NZ	2.25	0.51
1:A:435:LEU:O	1:A:438:LYS:HB2	2.11	0.51
1:A:301:LYS:HZ2	1:B:467:PRO:HD2	1.75	0.51
1:A:342:SER:O	1:A:343:GLU:HB2	2.11	0.51
1:A:404:LYS:N	1:A:405:PRO:HD2	2.26	0.51
1:A:238:THR:HG22	1:A:240:LYS:HG2	1.92	0.51
1:A:290:VAL:HG13	1:A:468:LEU:HD23	1.92	0.50
1:A:447:THR:O	1:A:451:GLN:HB2	2.11	0.50
1:A:301:LYS:HZ1	1:B:467:PRO:HD2	1.77	0.49
1:B:252:MET:SD	1:B:277:VAL:HG11	2.52	0.49
1:B:382:SER:OG	1:B:420:GLN:NE2	2.46	0.49
1:B:437:GLN:O	1:B:440:THR:HG23	2.13	0.48
1:B:363:PHE:HZ	1:B:453:LEU:CD1	2.22	0.48
1:B:472:ILE:CG2	1:B:472:ILE:O	2.62	0.48
1:B:319:LYS:HE3	1:B:472:ILE:HG23	1.95	0.48
1:B:321:GLY:O	1:B:325:ILE:HG12	2.14	0.48
1:A:288:ARG:HA	1:A:288:ARG:HD2	1.64	0.47
1:B:365:GLU:N	1:B:366:PRO:CD	2.77	0.47
1:A:275:LYS:HB3	1:A:276:GLU:H	1.54	0.47
1:B:318:LEU:O	1:B:322:VAL:HG23	2.14	0.47
1:B:384:LEU:O	1:B:388:ILE:HG12	2.16	0.46
1:A:411:ASP:O	1:A:415:GLN:HG3	2.16	0.46
1:A:275:LYS:HG3	1:A:283:GLN:HE22	1.80	0.46
1:A:258:GLY:O	1:A:261:LYS:HB3	2.16	0.45
1:A:272:GLU:O	1:A:274:SER:N	2.48	0.45
2:A:101:SP3:H34	2:A:101:SP3:N11	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:THR:HG21	1:A:240:LYS:HG2	1.98	0.45
1:B:282:PHE:CE1	2:B:201:SP3:H30	2.52	0.45
1:A:291:GLU:O	1:A:295:GLU:HG3	2.16	0.45
1:A:232:LYS:O	1:A:236:ILE:HG12	2.16	0.45
1:B:402:ASN:N	1:B:402:ASN:ND2	2.63	0.45
1:B:208:SER:O	1:B:212:ARG:HG2	2.16	0.45
1:B:342:SER:O	1:B:345:GLN:HB2	2.17	0.45
1:A:247:PHE:HZ	1:A:257:MET:CG	2.27	0.45
1:A:433:ALA:O	1:A:437:GLN:HG3	2.17	0.45
1:A:247:PHE:CZ	1:A:257:MET:CG	2.98	0.44
1:B:274:SER:O	1:B:275:LYS:CB	2.65	0.44
1:A:289:SER:O	1:A:293:VAL:HG23	2.16	0.44
1:A:438:LYS:HD3	1:A:438:LYS:HA	1.78	0.44
1:A:245:SER:HA	1:A:246:PRO:HD3	1.81	0.44
1:B:325:ILE:HD12	1:B:388:ILE:HD12	2.00	0.44
1:B:255:LEU:HD23	1:B:277:VAL:CG1	2.48	0.44
1:B:476:LEU:HB3	1:B:477:TYR:H	1.67	0.43
1:A:250:TYR:HA	1:A:352:PHE:HB2	2.00	0.43
1:B:273:GLN:OE1	1:B:273:GLN:HA	2.19	0.43
1:B:264:PHE:O	1:B:265:LYS:C	2.56	0.43
1:A:340:LEU:HB3	1:A:344:GLY:HA2	2.01	0.43
1:B:310:ASP:OD1	1:B:312:ASN:N	2.51	0.43
1:A:244:LYS:HB2	1:A:245:SER:H	1.53	0.42
1:B:230:LYS:O	1:B:234:ARG:HG2	2.19	0.42
1:A:265:LYS:NZ	1:A:345:GLN:HG3	2.35	0.42
1:B:255:LEU:HD23	1:B:277:VAL:HG13	2.02	0.42
1:A:279:ILE:HG22	1:A:283:GLN:HE22	1.83	0.42
1:A:469:LEU:O	1:A:472:ILE:HG22	2.18	0.42
1:A:307:VAL:HG22	3:A:80:HOH:O	2.19	0.42
1:A:261:LYS:HZ1	1:A:262:ILE:HD13	1.84	0.42
1:A:402:ASN:HD22	1:A:402:ASN:HA	1.65	0.42
1:A:268:THR:HB	1:A:269:PRO:HD2	2.01	0.42
1:A:362:ASP:OD1	1:A:362:ASP:N	2.53	0.42
1:A:268:THR:O	1:A:270:LEU:N	2.52	0.41
1:B:392:ILE:HG22	1:B:393:LEU:HD22	2.02	0.41
1:A:365:GLU:HB3	1:A:366:PRO:HD3	2.02	0.41
1:A:327:TYR:CE2	1:A:446:VAL:HG22	2.55	0.41
1:A:249:ILE:HG23	1:A:255:LEU:HA	2.01	0.41
1:A:317:LEU:HD11	1:A:406:ILE:HG12	2.01	0.41
1:B:421:LEU:HD11	1:B:435:LEU:HD23	2.03	0.41
1:B:232:LYS:NZ	3:B:76:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASP:HA	1:B:264:PHE:HB3	2.03	0.41
1:B:271:GLN:NE2	1:B:271:GLN:CA	2.76	0.41
1:B:293:VAL:CG2	1:B:322:VAL:HG11	2.44	0.41
1:A:368:PHE:O	1:A:372:VAL:HG23	2.21	0.41
1:A:299:TYR:CE2	1:A:388:ILE:HG22	2.56	0.41
1:A:219:TYR:O	1:A:223:ILE:HG12	2.21	0.41
1:A:363:PHE:HE1	1:A:449:HIS:CE1	2.38	0.40
1:B:289:SER:O	1:B:293:VAL:HG23	2.22	0.40
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.52	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	269/271 (99%)	228 (85%)	31 (12%)	10 (4%)	3	2
1	B	269/271 (99%)	242 (90%)	26 (10%)	1 (0%)	34	42
All	All	538/542 (99%)	470 (87%)	57 (11%)	11 (2%)	7	6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
1	A	262	ILE
1	A	277	VAL
1	A	453	LEU
1	B	239	GLY
1	A	349	THR
1	A	359	PRO
1	A	464	SER
1	A	245	SER

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Mol	Chain	Res	Type
1	A	269	PRO
1	A	358	LYS

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	244/244 (100%)	218 (89%)	26 (11%)	6	7
1	B	244/244 (100%)	223 (91%)	21 (9%)	10	12
All	All	488/488 (100%)	441 (90%)	47 (10%)	8	10

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	220	ASP
1	A	221	SER
1	A	244	LYS
1	A	261	LYS
1	A	268	THR
1	A	271	GLN
1	A	275	LYS
1	A	283	GLN
1	A	288	ARG
1	A	336	LYS
1	A	342	SER
1	A	345	GLN
1	A	362	ASP
1	A	363	PHE
1	A	388	ILE
1	A	402	ASN
1	A	411	ASP
1	A	441	ASP
1	A	452	LEU
1	A	456	ILE

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Mol	Chain	Res	Type
1	A	463	MET
1	A	472	ILE
1	A	474	LYS
1	A	476	LEU
1	A	477	TYR
1	B	223	ILE
1	B	224	LYS
1	B	244	LYS
1	B	245	SER
1	B	257	MET
1	B	260	ASP
1	B	270	LEU
1	B	271	GLN
1	B	275	LYS
1	B	288	ARG
1	B	318	LEU
1	B	363	PHE
1	B	382	SER
1	B	428	SER
1	B	440	THR
1	B	453	LEU
1	B	461	THR
1	B	464	SER
1	B	465	LEU
1	B	469	LEU
1	B	474	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	294	GLN
1	A	308	ASN
1	A	312	ASN
1	A	402	ASN
1	A	412	ASN
1	A	437	GLN
1	A	451	GLN
1	B	271	GLN
1	B	283	GLN
1	B	286	GLN
1	B	402	ASN

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Mol	Chain	Res	Type
1	B	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SP3	A	101	-	37,38,38	2.44	9 (24%)	47,59,59	2.35	13 (27%)
2	SP3	B	201	-	37,38,38	2.42	9 (24%)	47,59,59	2.12	11 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SP3	A	101	-	-	3/26/31/31	0/4/4/4
2	SP3	B	201	-	-	3/26/31/31	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	SP3	N7-N8	-8.09	1.23	1.39
2	B	201	SP3	N7-N8	-7.98	1.23	1.39
2	B	201	SP3	O14-S12	6.59	1.51	1.43
2	A	101	SP3	O14-S12	6.46	1.50	1.43
2	B	201	SP3	O13-S12	5.80	1.50	1.43
2	A	101	SP3	O13-S12	5.79	1.50	1.43
2	A	101	SP3	C6-C3	-4.13	1.39	1.49
2	B	201	SP3	C6-C3	-3.73	1.40	1.49
2	A	101	SP3	C10-C6	-3.66	1.33	1.40
2	B	201	SP3	C9-N8	-3.47	1.33	1.37
2	B	201	SP3	C10-C6	-3.41	1.34	1.40
2	A	101	SP3	C29-N8	-3.35	1.34	1.44
2	B	201	SP3	C29-N8	-3.27	1.34	1.44
2	A	101	SP3	C9-N8	-3.26	1.33	1.37
2	A	101	SP3	C15-S12	-2.81	1.72	1.76
2	B	201	SP3	C25-C19	2.44	1.55	1.49
2	A	101	SP3	C25-C19	2.27	1.54	1.49
2	B	201	SP3	C21-C17	2.23	1.54	1.49

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	SP3	C1-C5-S4	-9.68	105.12	112.98
2	B	201	SP3	O14-S12-O13	-7.96	109.76	119.55
2	B	201	SP3	C1-C5-S4	-5.88	108.21	112.98
2	A	101	SP3	O14-S12-O13	-5.73	112.50	119.55
2	A	101	SP3	O13-S12-C15	4.74	113.81	107.97
2	B	201	SP3	C3-C6-N7	3.99	127.47	120.88
2	B	201	SP3	C19-C20-C15	3.92	121.96	118.95
2	A	101	SP3	C18-C17-C21	3.35	124.10	119.58
2	A	101	SP3	F24-C21-C17	-3.31	105.66	112.93
2	A	101	SP3	C16-C17-C21	-3.29	115.14	119.58
2	B	201	SP3	C29-N8-C9	-3.28	125.21	129.11
2	A	101	SP3	C16-C15-S12	-3.12	115.58	119.08
2	A	101	SP3	C20-C15-S12	3.01	122.44	119.08
2	B	201	SP3	O13-S12-C15	2.96	111.61	107.97
2	A	101	SP3	F28-C25-C19	-2.82	106.74	112.93
2	B	201	SP3	C10-C6-C3	-2.75	125.32	129.32
2	A	101	SP3	C3-C6-N7	2.70	125.34	120.88
2	B	201	SP3	F26-C25-F28	2.54	115.04	105.72
2	B	201	SP3	F22-C21-F24	2.38	114.44	105.72
2	A	101	SP3	C29-N8-C9	-2.37	126.30	129.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	SP3	C15-S12-N11	2.21	109.62	106.83
2	B	201	SP3	C16-C15-S12	2.18	121.51	119.08
2	A	101	SP3	F26-C25-F28	2.12	113.48	105.72
2	A	101	SP3	F23-C21-F22	2.08	113.36	105.72

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	SP3	S4-C3-C6-C10
2	B	201	SP3	S4-C3-C6-C10
2	B	201	SP3	C30-C29-N8-C9
2	B	201	SP3	C34-C29-N8-C9
2	A	101	SP3	C34-C29-N8-C9
2	A	101	SP3	C30-C29-N8-C9

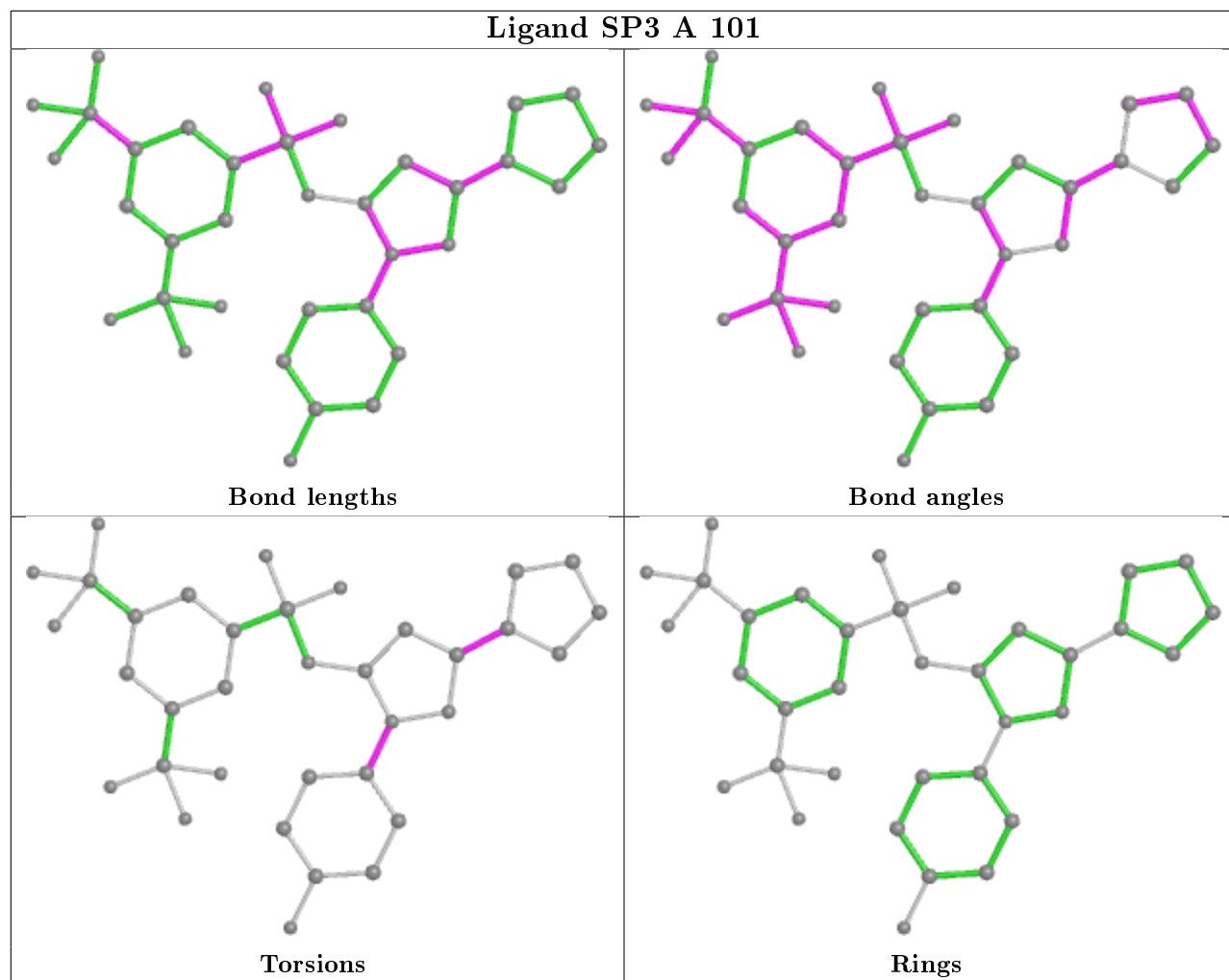
There are no ring outliers.

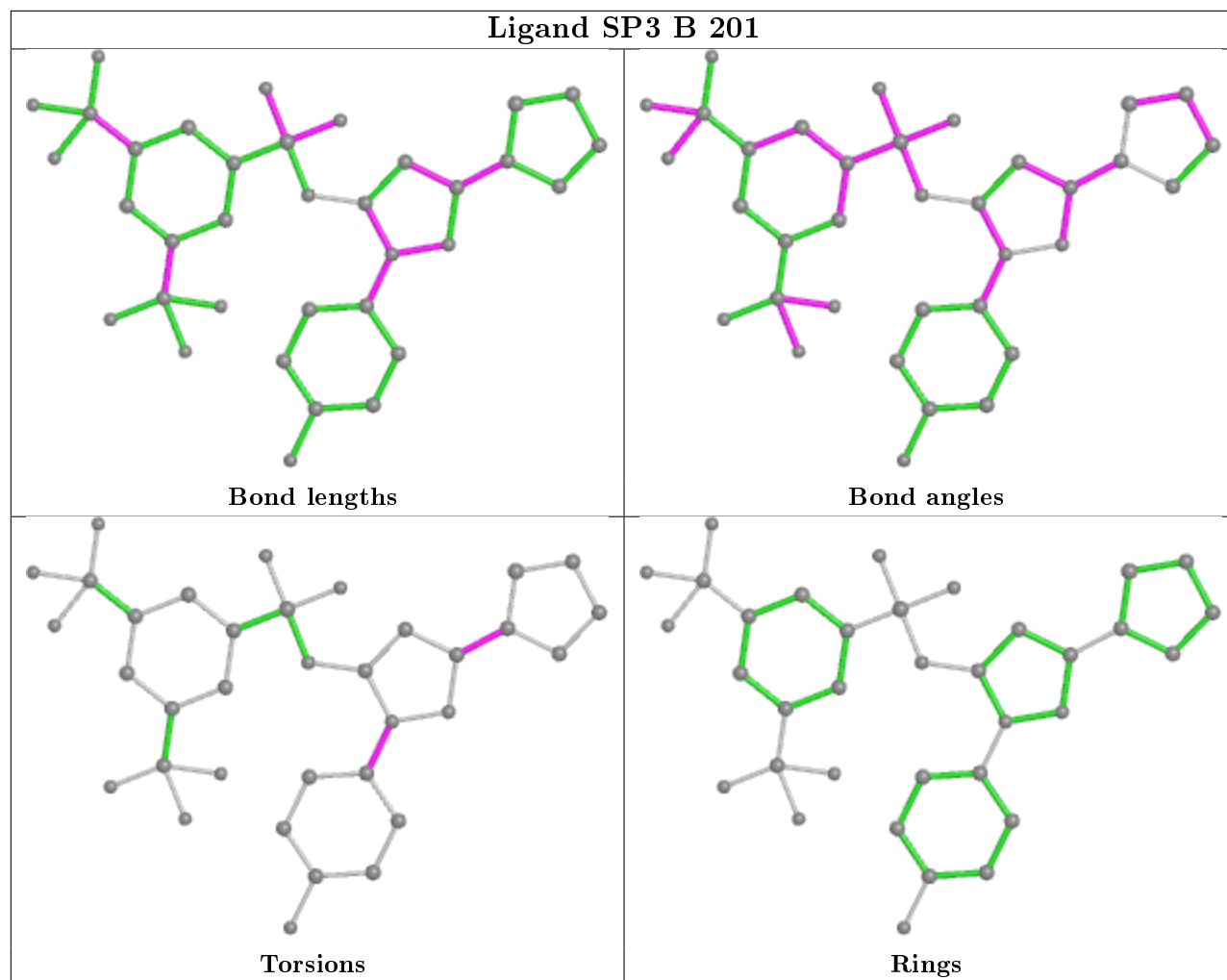
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	SP3	4	0
2	B	201	SP3	4	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.

Ligand SP3 A 101





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	271/271 (100%)	0.67	39 (14%) 2 3	23, 45, 119, 133	0
1	B	271/271 (100%)	0.48	32 (11%) 4 6	17, 34, 104, 122	0
All	All	542/542 (100%)	0.58	71 (13%) 3 4	17, 39, 109, 133	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	ILE	15.6
1	B	476	LEU	11.5
1	A	267	ILE	11.4
1	B	468	LEU	11.3
1	B	474	LYS	10.0
1	B	477	TYR	9.6
1	A	270	LEU	9.2
1	A	263	LYS	8.9
1	B	241	THR	8.4
1	B	473	TYR	8.4
1	B	470	GLN	7.4
1	B	266	HIS	6.7
1	B	469	LEU	6.7
1	A	477	TYR	6.2
1	A	264	PHE	6.2
1	A	269	PRO	6.1
1	A	242	THR	6.1
1	B	260	ASP	6.0
1	B	465	LEU	5.7
1	A	271	GLN	5.5
1	A	266	HIS	5.5
1	B	467	PRO	5.4
1	B	471	GLU	5.2
1	A	268	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	463	MET	5.1
1	B	265	LYS	5.0
1	B	243	ASP	4.9
1	A	272	GLU	4.9
1	A	283	GLN	4.7
1	B	268	THR	4.6
1	B	273	GLN	4.6
1	B	472	ILE	4.4
1	A	459	THR	4.3
1	A	252	MET	4.2
1	B	269	PRO	4.2
1	A	262	ILE	4.1
1	B	240	LYS	4.0
1	A	358	LYS	3.9
1	A	461	THR	3.9
1	B	463	MET	3.7
1	A	250	TYR	3.7
1	A	255	LEU	3.7
1	B	242	THR	3.7
1	B	264	PHE	3.7
1	A	462	ASP	3.5
1	A	277	VAL	3.5
1	A	273	GLN	3.4
1	A	265	LYS	3.4
1	B	262	ILE	3.3
1	B	261	LYS	3.2
1	A	241	THR	3.1
1	A	341	ILE	3.0
1	B	358	LYS	2.9
1	A	245	SER	2.8
1	B	466	HIS	2.8
1	A	281	ILE	2.6
1	A	239	GLY	2.6
1	A	259	GLU	2.5
1	A	238	THR	2.4
1	B	244	LYS	2.4
1	A	261	LYS	2.4
1	A	240	LYS	2.3
1	B	475	ASP	2.3
1	A	340	LEU	2.2
1	B	464	SER	2.2
1	B	270	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	258	GLY	2.2
1	A	249	ILE	2.2
1	A	285	CYS	2.1
1	A	251	ASP	2.1
1	A	470	GLN	2.1

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](#)

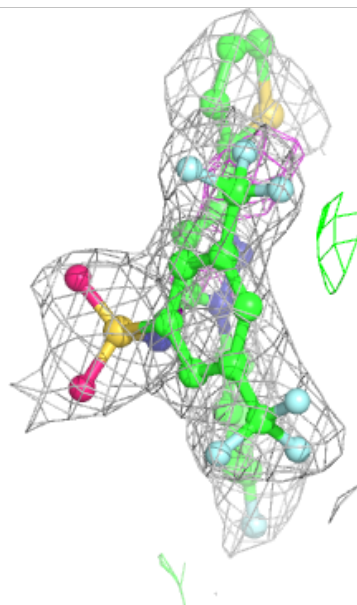
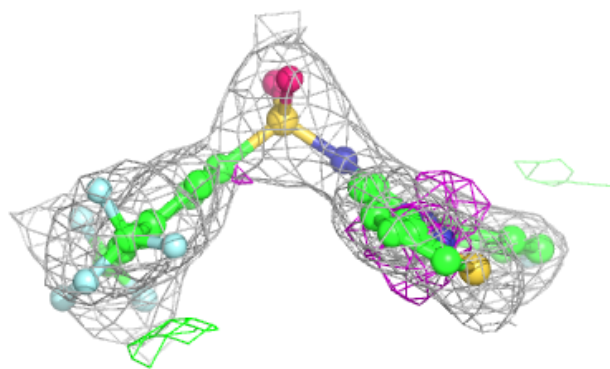
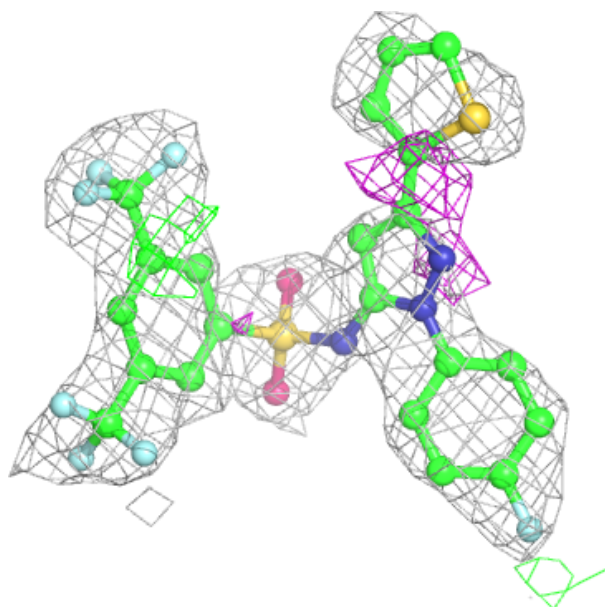
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SP3	B	201	35/35	0.87	0.18	49,60,67,71	0
2	SP3	A	101	35/35	0.91	0.19	55,65,72,74	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.

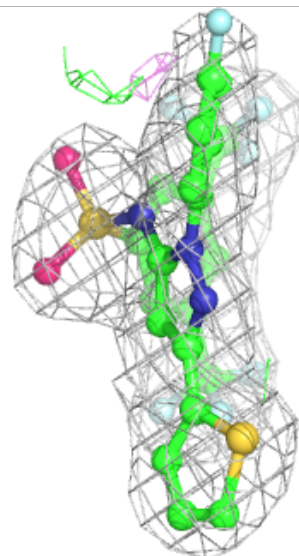
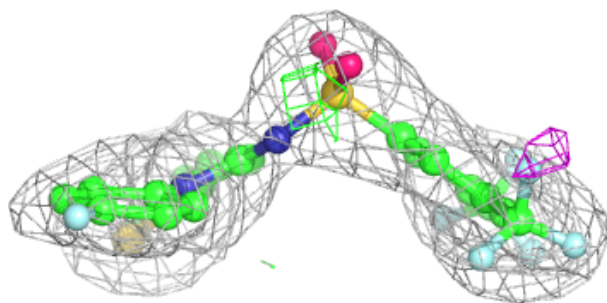
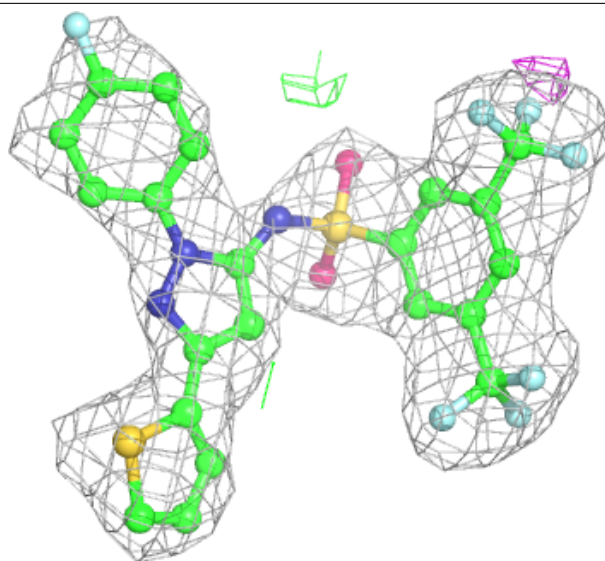
Electron density around SP3 B 201:

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



Electron density around SP3 A 101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.