Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:10 am BST

PDB ID	:	5F9B
Title	:	X-ray crystal structure of PPARgamma in the complex with caulophyllogenin
Authors	:	Pochetti, G.; Montanari, R.; Capelli, D.
Deposited on	:	2015-12-09
Resolution	:	2.25 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:

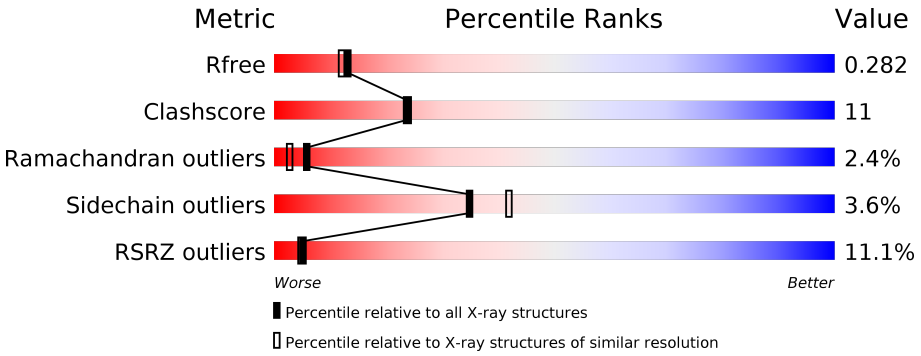
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	287	8% 68% 19% • 11%
1	B	287	12% 65% 19% •• 13%

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	5VN	B	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4155 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.

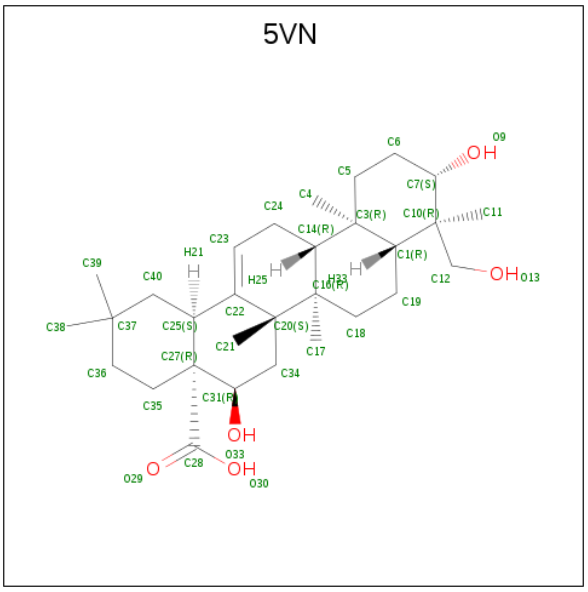
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2029	1310	331	378	10			
1	B	250	Total	C	N	O	S	0	0	0
			1993	1288	323	372	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	expression tag	UNP P37231
A	192	SER	-	expression tag	UNP P37231
A	193	HIS	-	expression tag	UNP P37231
A	194	MET	-	expression tag	UNP P37231
B	191	GLY	-	expression tag	UNP P37231
B	192	SER	-	expression tag	UNP P37231
B	193	HIS	-	expression tag	UNP P37231
B	194	MET	-	expression tag	UNP P37231

- Molecule 2 is Caulophyllogenin (three-letter code: 5VN) (formula: $C_{30}H_{48}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 35 30 5	0	0

- Molecule 3 is water.

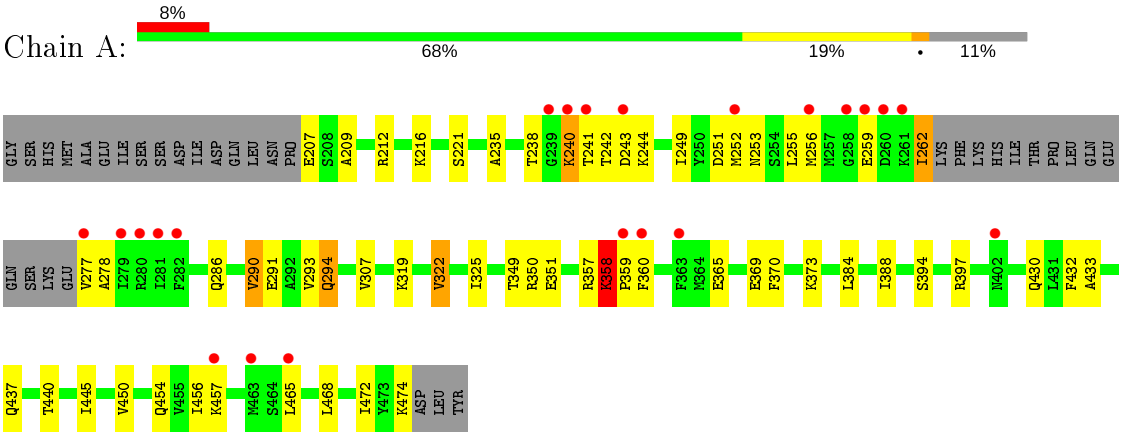
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	B	43	Total O 43 43	0	0

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.

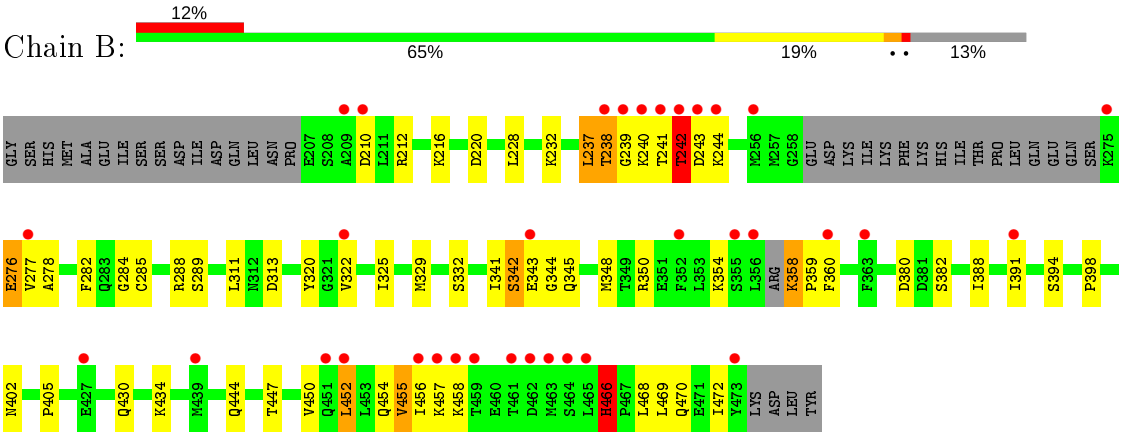
- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain A:



- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.21Å 61.66Å 118.90Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	45.91 – 2.25 45.91 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.91-2.25) 99.1 (45.91-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.230 , 0.281 0.231 , 0.282	Depositor DCC
R_{free} test set	1549 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4155	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 5VN

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	0.47	0/2062	0.62	1/2778 (0.0%)
1	B	0.48	0/2026	0.65	2/2731 (0.1%)
All	All	0.48	0/4088	0.64	3/5509 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	358	LYS	C-N-CD	6.97	143.05	128.40
1	B	239	GLY	N-CA-C	-6.74	96.26	113.10
1	B	455	VAL	N-CA-C	-5.55	96.02	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	238	THR	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	2029	0	2092	43	0
1	B	1993	0	2051	48	0
2	B	35	0	0	9	0
3	A	55	0	0	6	0
3	B	43	0	0	3	0
All	All	4155	0	4143	91	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 11.

All (91) 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:262:ILE:HA	3:A:533:HOH:O	1.60	0.99
1:A:358:LYS:HB3	1:A:359:PRO:HD3	1.52	0.89
1:A:277:VAL:N	3:A:502:HOH:O	2.09	0.84
1:B:285:CYS:HA	2:B:501:5VN:C21	2.12	0.80
1:B:455:VAL:O	1:B:458:LYS:HB2	1.88	0.73
1:B:342:SER:N	2:B:501:5VN:O29	2.19	0.73
1:B:243:ASP:OD1	1:B:244:LYS:N	2.22	0.72
1:A:253:ASN:HA	1:A:256:MET:HG3	1.71	0.72
1:B:358:LYS:HB3	1:B:359:PRO:HD2	1.69	0.72
1:A:235:ALA:HA	1:A:240:LYS:HD3	1.73	0.71
1:A:242:THR:O	3:A:501:HOH:O	2.08	0.70
1:B:212:ARG:NH1	3:B:602:HOH:O	2.21	0.70
1:A:358:LYS:HB3	1:A:359:PRO:CD	2.22	0.68
1:B:341:ILE:HG12	2:B:501:5VN:O30	1.92	0.68
1:A:349:THR:HG22	1:A:351:GLU:H	1.60	0.66
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.77	0.66
1:B:313:ASP:OD2	3:B:601:HOH:O	2.14	0.65
1:B:455:VAL:HA	1:B:458:LYS:HG2	1.79	0.64
1:A:207:GLU:HG3	1:A:209:ALA:H	1.65	0.62
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.30	0.61
1:A:241:THR:HG22	1:A:243:ASP:OD2	2.02	0.60
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LYS:HB2	1:B:360:PHE:HD2	1.66	0.60
1:B:240:LYS:O	1:B:242:THR:N	2.35	0.59
1:A:243:ASP:O	1:A:244:LYS:HG2	2.03	0.58
1:B:342:SER:C	1:B:343:GLU:HG3	2.25	0.56
1:B:228:LEU:HD12	1:B:232:LYS:HG2	1.88	0.56
1:A:430:GLN:HG3	1:A:433:ALA:HB3	1.90	0.54
1:A:349:THR:HG22	1:A:351:GLU:N	2.23	0.53
1:A:319:LYS:NZ	1:A:474:LYS:HG2	2.24	0.52
1:B:341:ILE:HA	2:B:501:5VN:O30	2.08	0.52
1:A:433:ALA:O	1:A:437:GLN:HG3	2.09	0.52
1:A:359:PRO:HB2	1:A:456:ILE:HD11	1.91	0.52
1:B:466:HIS:HB3	1:B:469:LEU:HB3	1.92	0.52
1:A:293:VAL:HG11	1:A:468:LEU:HD11	1.93	0.50
1:B:282:PHE:O	1:B:285:CYS:HB2	2.10	0.50
1:A:252:MET:O	1:A:255:LEU:HB3	2.12	0.50
1:B:469:LEU:HD12	1:B:472:ILE:HD12	1.94	0.50
1:B:452:LEU:O	1:B:456:ILE:HG12	2.11	0.50
1:A:350:ARG:NH2	1:A:365:GLU:OE2	2.39	0.49
1:A:286:GLN:CD	1:A:465:LEU:HD12	2.33	0.49
1:B:466:HIS:CD2	3:B:607:HOH:O	2.66	0.49
1:B:402:ASN:O	1:B:405:PRO:HD2	2.13	0.49
1:A:357:ARG:HD2	3:A:507:HOH:O	2.14	0.48
1:B:284:GLY:HA3	2:B:501:5VN:C39	2.42	0.48
1:A:359:PRO:HD2	1:A:360:PHE:CD1	2.49	0.48
1:B:288:ARG:HG2	2:B:501:5VN:C34	2.44	0.47
1:B:341:ILE:CD1	1:B:348:MET:HB2	2.43	0.47
1:B:341:ILE:HA	2:B:501:5VN:C28	2.45	0.47
1:B:444:GLN:HA	1:B:447:THR:HB	1.95	0.47
1:A:242:THR:O	1:A:242:THR:OG1	2.24	0.47
1:B:342:SER:C	1:B:344:GLY:H	2.19	0.47
1:B:452:LEU:C	1:B:454:GLN:H	2.17	0.46
1:A:394:SER:HB2	1:A:397:ARG:HG2	1.96	0.46
1:A:450:VAL:O	1:A:454:GLN:HG3	2.15	0.46
1:A:322:VAL:HG11	1:A:472:ILE:HD13	1.98	0.46
1:A:384:LEU:O	1:A:388:ILE:HG12	2.16	0.46
1:A:319:LYS:HZ3	1:A:474:LYS:HG2	1.79	0.46
1:B:276:GLU:O	1:B:278:ALA:N	2.49	0.46
1:A:290:VAL:O	1:A:294:GLN:HG2	2.15	0.46
1:B:430:GLN:O	1:B:434:LYS:HG3	2.16	0.45
1:B:452:LEU:HA	1:B:455:VAL:HG23	1.99	0.45
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ARG:HB3	2:B:501:5VN:C21	2.46	0.45
1:A:307:VAL:HG22	3:A:513:HOH:O	2.17	0.45
1:A:212:ARG:HD2	1:A:212:ARG:HA	1.78	0.44
1:B:343:GLU:HB2	1:B:345:GLN:HG3	1.98	0.44
1:B:447:THR:O	1:B:450:VAL:HG22	2.17	0.44
1:A:437:GLN:O	1:A:440:THR:HG22	2.18	0.44
1:B:325:ILE:HD11	1:B:391:ILE:HB	1.99	0.44
1:A:216:LYS:HD2	1:A:216:LYS:HA	1.86	0.43
1:B:216:LYS:NZ	1:B:220:ASP:OD1	2.51	0.43
1:B:468:LEU:HD12	1:B:468:LEU:HA	1.84	0.43
1:B:380:ASP:OD1	1:B:382:SER:OG	2.24	0.43
1:B:444:GLN:O	1:B:444:GLN:HG2	2.18	0.43
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.54	0.42
1:A:277:VAL:HG13	1:A:278:ALA:N	2.33	0.42
1:B:350:ARG:O	1:B:354:LYS:HG3	2.20	0.42
1:A:286:GLN:O	1:A:290:VAL:HG12	2.20	0.42
1:B:237:LEU:HA	1:B:237:LEU:HD23	1.89	0.42
1:A:369:GLU:O	1:A:373:LYS:HG3	2.20	0.42
1:A:432:PHE:HB3	3:A:517:HOH:O	2.20	0.41
1:B:289:SER:HB3	2:B:501:5VN:C12	2.50	0.41
1:A:370:PHE:HB2	1:A:445:ILE:HD11	2.02	0.41
1:B:329:MET:O	1:B:332:SER:HB2	2.20	0.41
1:A:207:GLU:HG3	1:A:209:ALA:N	2.34	0.41
1:B:455:VAL:O	1:B:458:LYS:CB	2.65	0.41
1:B:341:ILE:O	1:B:342:SER:O	2.39	0.41
1:A:291:GLU:O	1:A:294:GLN:HG3	2.21	0.41
1:B:237:LEU:HB3	1:B:238:THR:H	1.60	0.41
1:A:325:ILE:HD13	1:A:388:ILE:HG23	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	250/287 (87%)	240 (96%)	7 (3%)	3 (1%)	13 9
1	B	246/287 (86%)	226 (92%)	11 (4%)	9 (4%)	3 1
All	All	496/574 (86%)	466 (94%)	18 (4%)	12 (2%)	6 3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	B	237	LEU
1	B	241	THR
1	B	242	THR
1	B	358	LYS
1	B	276	GLU
1	B	277	VAL
1	B	342	SER
1	B	394	SER
1	A	238	THR
1	A	240	LYS
1	B	466	HIS

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	227/258 (88%)	219 (96%)	8 (4%)	36 43
1	B	223/258 (86%)	215 (96%)	8 (4%)	35 42
All	All	450/516 (87%)	434 (96%)	16 (4%)	35 42

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	SER
1	A	251	ASP
1	A	259	GLU
1	A	262	ILE

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Mol	Chain	Res	Type
1	A	290	VAL
1	A	294	GLN
1	A	322	VAL
1	A	457	LYS
1	B	210	ASP
1	B	242	THR
1	B	311	LEU
1	B	322	VAL
1	B	452	LEU
1	B	457	LYS
1	B	466	HIS
1	B	470	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	B	444	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)

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	$\#\|Z\| > 2$
2	5VN	B	501	-	37,39,39	1.72	7 (18%)	55,68,68	2.64	23 (41%)

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	5VN	B	501	-	-	0/3/104/104	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	5VN	C3-C14	-4.48	1.49	1.56
2	B	501	5VN	C16-C20	-3.87	1.52	1.58
2	B	501	5VN	C27-C31	-3.79	1.49	1.55
2	B	501	5VN	C34-C20	-3.20	1.47	1.54
2	B	501	5VN	C23-C22	2.86	1.38	1.33
2	B	501	5VN	C34-C31	2.82	1.58	1.53
2	B	501	5VN	C5-C3	-2.29	1.50	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	5VN	C21-C20-C16	-10.61	102.42	112.33
2	B	501	5VN	C20-C16-C14	-7.46	97.17	108.04
2	B	501	5VN	C37-C40-C25	-4.10	108.55	114.38
2	B	501	5VN	C21-C20-C22	3.91	111.03	106.95
2	B	501	5VN	C25-C22-C23	-3.74	114.15	118.92
2	B	501	5VN	C14-C24-C23	-3.74	106.05	113.02
2	B	501	5VN	C4-C3-C14	-3.55	106.34	112.92
2	B	501	5VN	C17-C16-C14	3.35	116.86	111.91
2	B	501	5VN	C16-C20-C22	3.17	112.87	108.80
2	B	501	5VN	C10-C1-C3	-2.97	113.08	117.03
2	B	501	5VN	C24-C23-C22	-2.91	119.60	125.07
2	B	501	5VN	C4-C3-C1	2.86	118.22	112.92
2	B	501	5VN	O33-C31-C34	2.81	116.88	110.19
2	B	501	5VN	C39-C37-C38	-2.64	104.55	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	5VN	C35-C36-C37	-2.60	110.52	113.19
2	B	501	5VN	C24-C14-C3	-2.52	109.55	113.43
2	B	501	5VN	C17-C16-C20	2.51	112.93	109.97
2	B	501	5VN	C18-C16-C20	-2.51	107.64	110.26
2	B	501	5VN	C6-C7-C10	-2.45	110.52	113.15
2	B	501	5VN	C5-C6-C7	-2.41	107.87	111.51
2	B	501	5VN	C21-C20-C34	-2.27	104.30	108.52
2	B	501	5VN	C6-C5-C3	-2.14	109.11	112.78
2	B	501	5VN	O13-C12-C10	-2.12	109.57	113.11

There are no chirality outliers.

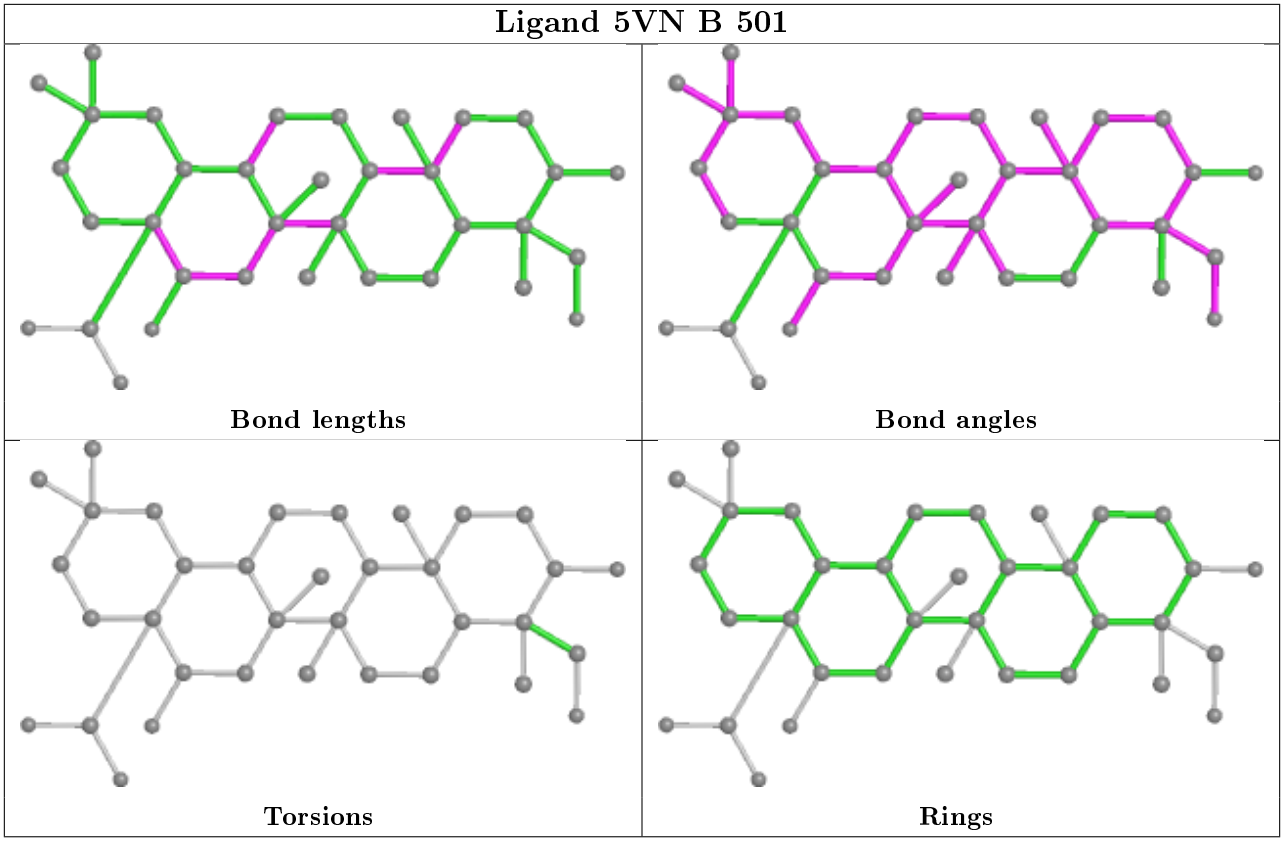
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	5VN	9	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 then 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^{th} 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	254/287 (88%)	0.55	22 (8%) 10 11	37, 54, 83, 102	0
1	B	250/287 (87%)	0.94	34 (13%) 3 2	39, 57, 105, 121	0
All	All	504/574 (87%)	0.74	56 (11%) 5 5	37, 55, 91, 121	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	462	ASP	9.4
1	B	464	SER	9.1
1	B	463	MET	8.8
1	B	242	THR	8.8
1	B	465	LEU	8.6
1	B	238	THR	8.3
1	B	461	THR	7.2
1	B	240	LYS	5.2
1	B	243	ASP	4.7
1	A	359	PRO	4.6
1	A	261	LYS	4.5
1	B	244	LYS	4.3
1	B	456	ILE	4.2
1	A	240	LYS	4.2
1	B	239	GLY	4.2
1	B	360	PHE	4.1
1	B	241	THR	4.0
1	A	252	MET	3.6
1	B	343	GLU	3.5
1	B	363	PHE	3.5
1	A	363	PHE	3.5
1	A	279	ILE	3.5
1	B	277	VAL	3.4
1	B	256	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	256	MET	3.4
1	A	259	GLU	3.3
1	B	452	LEU	3.3
1	B	209	ALA	3.2
1	B	458	LYS	3.2
1	A	465	LEU	3.1
1	B	427	GLU	3.1
1	B	451	GLN	3.0
1	A	277	VAL	3.0
1	A	239	GLY	2.9
1	B	356	LEU	2.9
1	A	258	GLY	2.9
1	A	360	PHE	2.8
1	B	355	SER	2.6
1	B	457	LYS	2.5
1	B	210	ASP	2.5
1	A	282	PHE	2.4
1	B	275	LYS	2.3
1	A	280	ARG	2.3
1	A	457	LYS	2.3
1	A	281	ILE	2.3
1	B	439	MET	2.2
1	A	241	THR	2.2
1	A	243	ASP	2.2
1	A	402	ASN	2.2
1	B	391	ILE	2.2
1	B	459	THR	2.1
1	B	322	VAL	2.1
1	B	473	TYR	2.1
1	B	352	PHE	2.1
1	A	260	ASP	2.0
1	A	463	MET	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)

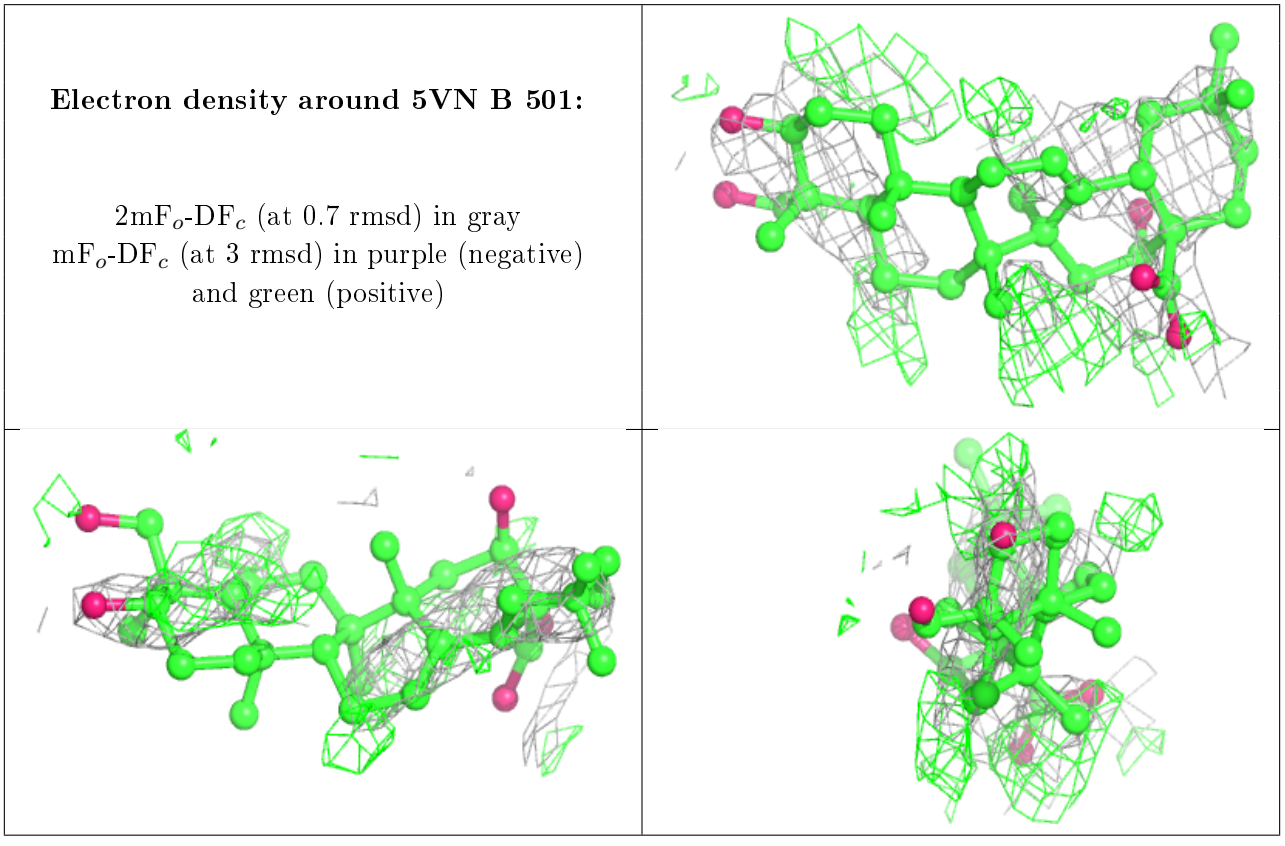
There are no carbohydrates in this entry.

6.4 Ligands

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^{th} 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^2)	Q<0.9
2	5VN	B	501	35/35	0.56	0.58	64,70,74,75	35

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.