



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:29 am BST

PDB ID : 3CFB  
Title : High-resolution structure of blue fluorescent antibody EP2-19G2 in complex with stilbene hapten at 100K  
Authors : Debler, E.W.; Wilson, I.A.  
Deposited on : 2008-03-03  
Resolution : 1.60 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

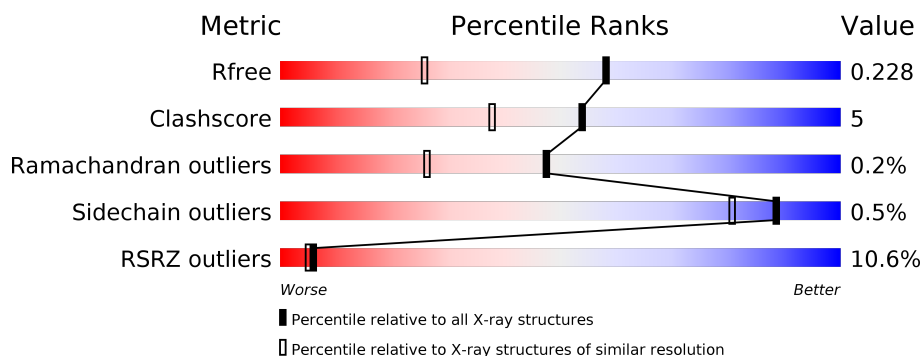
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	219	<div> <div>10%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	L	219	<div> <div>6%</div> <div>96%</div> <div>.</div> </div>
2	B	213	<div> <div>13%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	H	213	<div> <div>14%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7457 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.

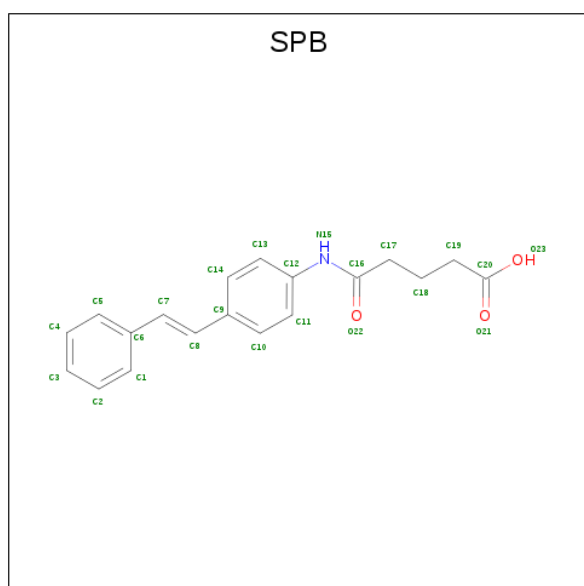
- Molecule 1 is a protein called BLUE FLUORESCENT ANTIBODY EP2-19G2-KAPPA LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	218	Total	C	N	O	S	0	9	0
			1745	1083	295	359	8			
1	A	218	Total	C	N	O	S	0	12	0
			1763	1095	295	363	10			

- Molecule 2 is a protein called BLUE FLUORESCENT ANTIBODY EP2-19G2-IGG2B HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	8	0
			1649	1036	275	329	9			
2	B	213	Total	C	N	O	S	0	5	0
			1628	1025	271	323	9			

- Molecule 3 is 4-(4-STYRYL-PHENYLCARBAMOYL)-BUTYRIC ACID (three-letter code: SPB) (formula: C<sub>19</sub>H<sub>19</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	N	O	0	0
			23	19	1	3		
3	B	1	Total	C	N	O	0	0
			23	19	1	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	171	Total	O	0	0
			171	171		
5	H	124	Total	O	0	0
			124	124		

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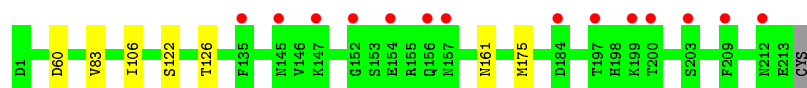
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	171	Total 171	O 171	0	0
5	B	124	Total 124	O 124	0	0

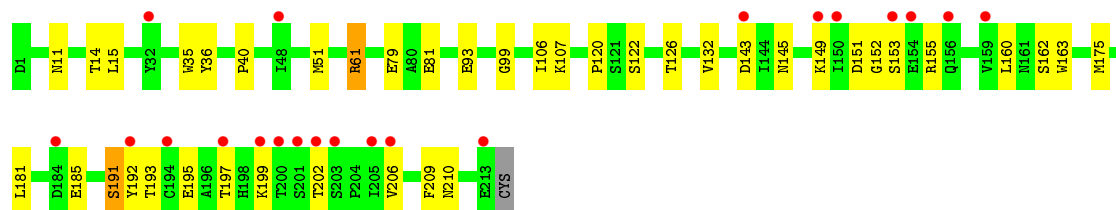
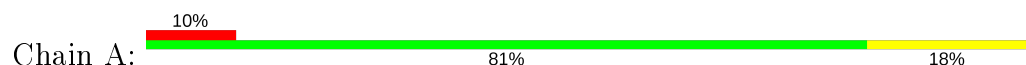
### 3 Residue-property plots [i](#)

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.

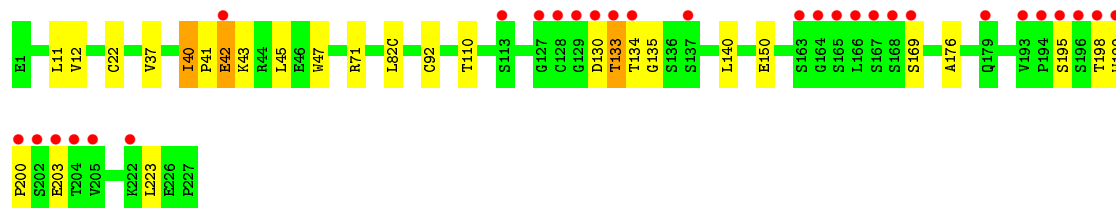
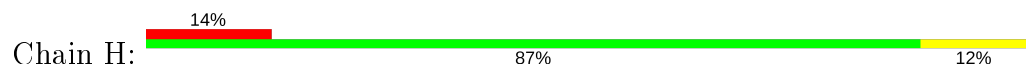
- Molecule 1: BLUE FLUORESCENT ANTIBODY EP2-19G2-KAPPA LIGHT CHAIN



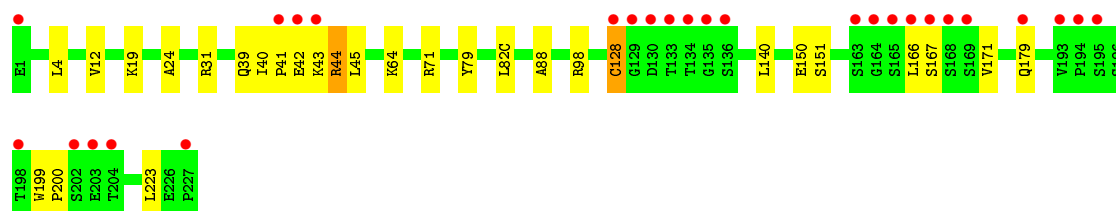
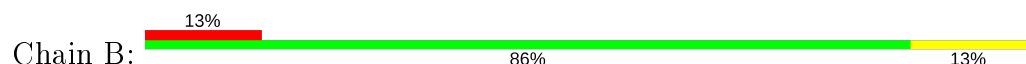
- Molecule 1: BLUE FLUORESCENT ANTIBODY EP2-19G2-KAPPA LIGHT CHAIN



- Molecule 2: BLUE FLUORESCENT ANTIBODY EP2-19G2-IGG2B HEAVY CHAIN



- Molecule 2: BLUE FLUORESCENT ANTIBODY EP2-19G2-IGG2B HEAVY CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.71Å 61.02Å 92.25Å 90.00° 116.65° 90.00°	Depositor
Resolution (Å)	42.03 – 1.60 42.04 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.03-1.60) 97.3 (42.04-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.3.0017	Depositor
R, $R_{free}$	0.186 , 0.218 0.195 , 0.228	Depositor DCC
$R_{free}$ test set	6274 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: GOL, SPB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.03	9/1800 (0.5%)	0.88	2/2445 (0.1%)
1	L	0.67	0/1782	0.75	1/2421 (0.0%)
2	B	0.63	0/1667	0.80	3/2273 (0.1%)
2	H	0.68	0/1688	0.79	3/2301 (0.1%)
All	All	0.77	9/6937 (0.1%)	0.81	9/9440 (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
2	B	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	SER	CB-OG	18.45	1.66	1.42
1	A	153	SER	C-O	7.51	1.37	1.23
1	A	93	GLU	CB-CG	-7.46	1.38	1.52
1	A	192	TYR	C-O	6.73	1.36	1.23
1	A	61	ARG	CB-CG	-6.50	1.34	1.52
1	A	210	ASN	CG-OD1	6.34	1.38	1.24
1	A	35	TRP	CE3-CZ3	5.82	1.48	1.38
1	A	93	GLU	CD-OE2	-5.74	1.19	1.25
1	A	36	TYR	CE2-CZ	-5.04	1.31	1.38

All (9) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	71	ARG	NE-CZ-NH1	7.63	124.12	120.30
2	B	71	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	61	ARG	CG-CD-NE	-6.99	97.11	111.80
1	A	151	ASP	CB-CG-OD2	-6.84	112.14	118.30
2	B	71	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	H	71	ARG	NE-CZ-NH2	-6.39	117.11	120.30
2	B	98	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	H	45	LEU	CA-CB-CG	5.61	128.19	115.30
1	L	60	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	166	LEU	Peptide
2	B	42	GLU	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1686	34	0
1	L	1745	0	1671	4	0
2	B	1628	0	1610	18	0
2	H	1649	0	1627	16	0
3	B	23	0	18	2	0
3	L	23	0	18	0	0
4	A	18	0	23	2	0
4	H	6	0	8	0	0
4	L	12	0	16	0	0
5	A	171	0	0	13	0
5	B	124	0	0	2	0
5	H	124	0	0	0	0
5	L	171	0	0	0	0
All	All	7457	0	6677	71	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 (71) 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:191:SER:CB	1:A:191:SER:OG	1.66	1.42
1:A:51[A]:MET:HE1	5:A:571:HOH:O	1.39	1.18
1:A:197:THR:HG23	5:A:535:HOH:O	1.64	0.96
1:A:15:LEU:HD21	1:A:106:ILE:HD13	1.61	0.79
1:A:15:LEU:CD2	1:A:106:ILE:HD13	2.19	0.72
2:B:31:ARG:HD2	5:B:400:HOH:O	1.92	0.68
2:H:140:LEU:HB3	2:H:223:LEU:CD2	2.27	0.65
1:A:191:SER:CB	1:A:191:SER:HG	2.09	0.63
1:A:14:THR:HG23	1:A:107:LYS:HE3	1.82	0.61
1:A:149:LYS:C	5:A:537:HOH:O	2.40	0.59
1:A:11:ASN:HB3	5:A:565:HOH:O	2.02	0.59
2:B:64:LYS:NZ	5:B:391:HOH:O	2.34	0.59
1:A:152:GLY:N	5:A:537:HOH:O	2.18	0.59
1:L:83:VAL:HG12	1:L:106:ILE:HG12	1.83	0.59
2:B:39:GLN:NE2	2:B:43:LYS:O	2.29	0.58
1:A:149:LYS:HB3	5:A:537:HOH:O	2.03	0.58
2:H:40:ILE:HG21	2:H:43:LYS:HD2	1.84	0.58
2:H:140:LEU:HB3	2:H:223:LEU:HD22	1.86	0.57
1:A:79:GLU:OE1	1:A:81:GLU:OE2	2.22	0.56
2:H:40:ILE:HG23	2:H:41:PRO:HD2	1.87	0.56
1:A:14:THR:CG2	1:A:107:LYS:HE3	2.36	0.55
4:A:404:GOL:H31	5:A:500:HOH:O	2.06	0.54
1:L:122:SER:O	1:L:126:THR:HG23	2.08	0.53
1:A:99:GLY:O	2:B:44:ARG:HG3	2.10	0.52
2:H:42:GLU:HG3	2:H:43:LYS:HG3	1.91	0.52
2:B:140:LEU:HB3	2:B:223:LEU:HD22	1.92	0.51
2:B:19:LYS:HE2	2:B:79:TYR:CD1	2.44	0.51
2:B:40:ILE:HG23	2:B:41:PRO:HD2	1.92	0.51
2:H:11:LEU:HD23	2:H:110:THR:HB	1.94	0.49
2:H:198:THR:O	2:H:203:GLU:N	2.45	0.49
1:A:191:SER:OG	1:A:191:SER:CA	2.53	0.49
2:B:39:GLN:NE2	2:B:40:ILE:O	2.40	0.48
2:H:150:GLU:OE2	2:H:176:ALA:HB3	2.13	0.48
1:A:143:ASP:HB2	1:A:199:LYS:HE3	1.96	0.48
1:A:155:ARG:CB	5:A:556:HOH:O	2.62	0.48
1:A:149:LYS:HA	5:A:556:HOH:O	2.13	0.47
2:B:45:LEU:HD11	3:B:302:SPB:C2	2.45	0.46
1:A:209:PHE:HB3	2:B:128:CYS:SG	2.55	0.46
2:H:37[B]:VAL:HG22	2:H:47:TRP:HA	1.97	0.46
1:A:193:THR:CG2	1:A:206:VAL:HG13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:ASP:O	2:H:133:THR:CB	2.63	0.46
1:A:122:SER:O	1:A:126:THR:HG23	2.15	0.46
2:H:22:CYS:SG	2:H:92[B]:CYS:CB	3.01	0.46
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.97	0.46
1:A:195:GLU:HB3	1:A:206:VAL:HG22	1.97	0.46
1:L:161:ASN:HB3	1:L:175:MET:HE3	1.98	0.45
2:H:12:VAL:HG11	2:H:82(C):LEU:HD13	1.98	0.45
2:B:12:VAL:HG11	2:B:82(C):LEU:HD13	2.00	0.44
2:B:4:LEU:HD23	2:B:24:ALA:HB2	2.00	0.44
1:L:83:VAL:CG1	1:L:106:ILE:HG12	2.48	0.43
1:A:149:LYS:CA	5:A:556:HOH:O	2.66	0.43
1:A:149:LYS:HB2	1:A:193:THR:HB	2.00	0.43
2:B:40:ILE:HG12	2:B:88:ALA:HB2	1.99	0.43
2:H:130:ASP:O	2:H:133:THR:HB	2.18	0.43
2:B:40:ILE:CG2	2:B:41:PRO:HD2	2.48	0.43
2:H:135:GLY:O	2:H:195:SER:HB2	2.19	0.43
1:A:155:ARG:HB3	5:A:556:HOH:O	2.19	0.43
1:A:160:LEU:HD11	2:B:179:GLN:HG3	2.00	0.42
2:H:133:THR:CG2	2:H:134:THR:N	2.82	0.42
2:B:150:GLU:HA	2:B:151:SER:HA	1.87	0.42
2:B:199:TRP:CG	2:B:200:PRO:HA	2.54	0.42
1:A:181:LEU:HD22	1:A:185:GLU:OE1	2.19	0.42
2:B:167:SER:HA	2:B:171:VAL:HG23	2.01	0.42
1:A:145:ASN:HB3	1:A:197:THR:OG1	2.20	0.41
1:A:162:SER:O	1:A:175[B]:MET:HG2	2.20	0.41
1:A:163:TRP:CD1	1:A:175[B]:MET:HG3	2.55	0.41
1:A:40:PRO:HG2	5:A:559:HOH:O	2.20	0.41
1:A:61:ARG:NH1	1:A:61:ARG:HG3	2.36	0.41
4:A:404:GOL:O3	3:B:302:SPB:O23	2.39	0.41
2:H:199:TRP:CD1	2:H:200:PRO:HA	2.56	0.40
1:A:202:THR:HG21	5:A:485:HOH:O	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	228/219 (104%)	223 (98%)	5 (2%)	0	100	100
1	L	225/219 (103%)	220 (98%)	5 (2%)	0	100	100
2	B	216/213 (101%)	208 (96%)	7 (3%)	1 (0%)	29	11
2	H	219/213 (103%)	212 (97%)	6 (3%)	1 (0%)	29	11
All	All	888/864 (103%)	863 (97%)	23 (3%)	2 (0%)	47	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	133	THR
2	B	128	CYS

### 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	205/194 (106%)	205 (100%)	0	100	100
1	L	202/194 (104%)	202 (100%)	0	100	100
2	B	189/184 (103%)	188 (100%)	1 (0%)	88	80
2	H	192/184 (104%)	189 (98%)	3 (2%)	62	41
All	All	788/756 (104%)	784 (100%)	4 (0%)	88	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	40	ILE
2	H	42	GLU
2	H	169	SER
2	B	44	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

### 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 ⓘ

8 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	$\# Z  > 2$
4	GOL	A	401	-	5,5,5	0.57	0	5,5,5	0.69	0
4	GOL	L	406	-	5,5,5	0.34	0	5,5,5	1.31	1 (20%)
4	GOL	A	403	-	5,5,5	0.71	0	5,5,5	0.44	0
4	GOL	L	402	-	5,5,5	0.36	0	5,5,5	0.46	0
4	GOL	H	405	-	5,5,5	0.27	0	5,5,5	0.76	0
3	SPB	B	302	-	21,24,24	0.72	0	26,30,30	1.08	1 (3%)
3	SPB	L	301	-	21,24,24	0.70	0	26,30,30	1.04	1 (3%)
4	GOL	A	404	-	5,5,5	0.91	0	5,5,5	1.51	1 (20%)

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
4	GOL	A	401	-	-	2/4/4/4	-
4	GOL	L	406	-	-	0/4/4/4	-
4	GOL	A	403	-	-	0/4/4/4	-
4	GOL	L	402	-	-	0/4/4/4	-
4	GOL	H	405	-	-	4/4/4/4	-
3	SPB	B	302	-	-	3/13/15/15	0/2/2/2
3	SPB	L	301	-	-	2/13/15/15	0/2/2/2
4	GOL	A	404	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	406	GOL	C3-C2-C1	-2.70	101.20	111.70
4	A	404	GOL	O3-C3-C2	-2.34	98.97	110.20
3	B	302	SPB	C13-C14-C9	2.19	124.11	121.25
3	L	301	SPB	C19-C18-C17	-2.14	107.30	114.34

There are no chirality outliers.

All (13) torsion outliers are listed below:

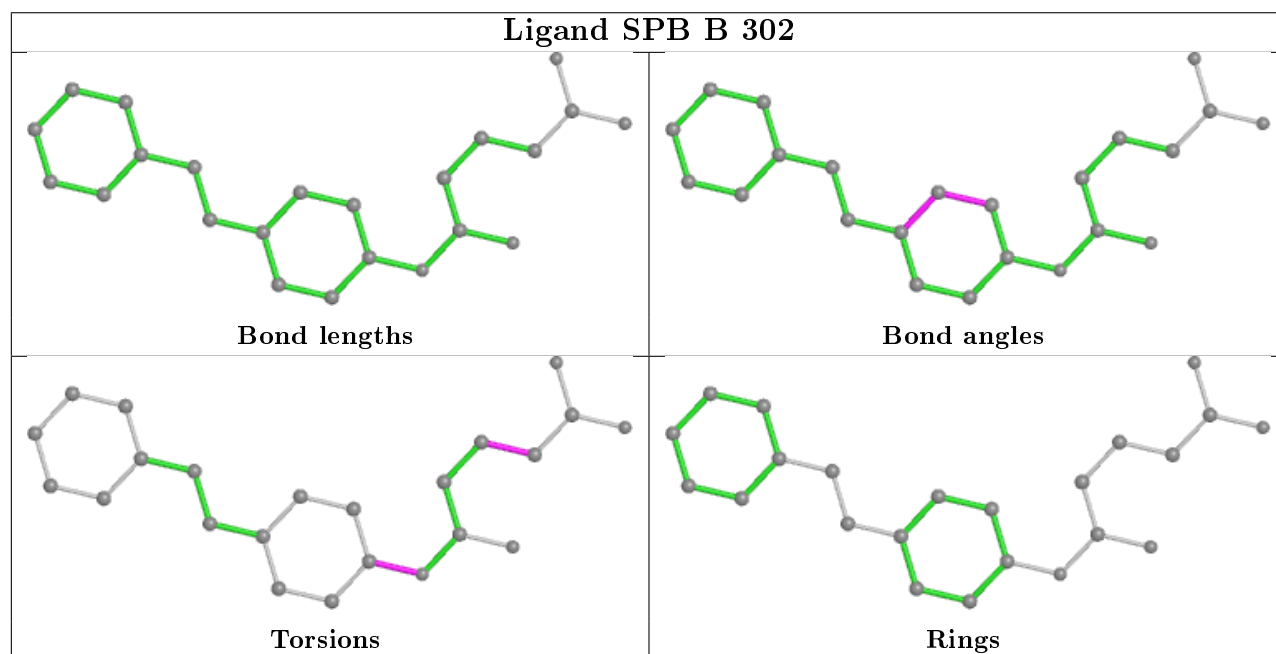
Mol	Chain	Res	Type	Atoms
4	H	405	GOL	C1-C2-C3-O3
3	B	302	SPB	C17-C18-C19-C20
4	A	404	GOL	O1-C1-C2-C3
4	A	401	GOL	O1-C1-C2-C3
4	H	405	GOL	O2-C2-C3-O3
4	A	404	GOL	O1-C1-C2-O2
4	A	401	GOL	O1-C1-C2-O2
3	L	301	SPB	C13-C12-N15-C16
4	H	405	GOL	O1-C1-C2-C3
4	H	405	GOL	O1-C1-C2-O2
3	B	302	SPB	C11-C12-N15-C16
3	B	302	SPB	C13-C12-N15-C16
3	L	301	SPB	C11-C12-N15-C16

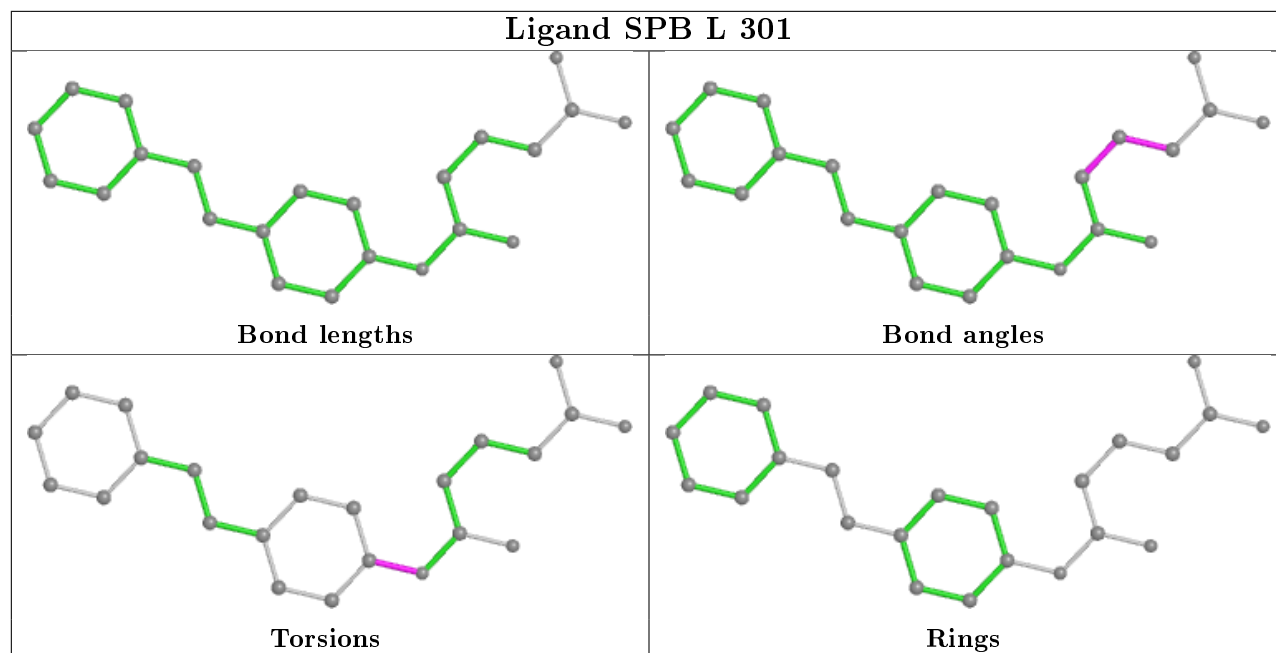
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	SPB	2	0
4	A	404	GOL	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	218/219 (99%)	0.66	21 (9%) 8 7	14, 20, 27, 35	0
1	L	218/219 (99%)	0.46	14 (6%) 19 17	17, 22, 29, 38	0
2	B	213/213 (100%)	0.76	27 (12%) 3 3	14, 21, 31, 38	0
2	H	213/213 (100%)	0.71	29 (13%) 3 2	16, 22, 32, 41	0
All	All	862/864 (99%)	0.65	91 (10%) 6 5	14, 21, 30, 41	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	128	CYS	12.1
2	B	130	ASP	11.8
2	B	133	THR	8.9
2	B	166	LEU	8.3
2	H	133	THR	7.9
2	H	128	CYS	6.5
2	H	129	GLY	6.1
2	B	163	SER	5.9
2	H	163	SER	5.8
2	B	165	SER	5.1
2	B	168	SER	5.1
2	H	164	GLY	4.9
2	H	194	PRO	4.7
2	H	202	SER	4.7
1	A	203	SER	4.6
2	B	198	THR	4.4
1	L	157	ASN	4.4
2	H	165	SER	4.3
2	H	198	THR	4.3
2	H	166	LEU	4.2
2	H	134	THR	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	227	PRO	4.1
1	A	154	GLU	4.1
2	B	203	GLU	3.9
2	B	204	THR	3.9
2	B	194	PRO	3.9
2	H	130	ASP	3.8
2	H	204	THR	3.8
2	B	193	VAL	3.7
2	B	129	GLY	3.7
2	B	167	SER	3.6
2	H	203	GLU	3.6
1	A	197	THR	3.4
1	L	147	LYS	3.4
2	B	202	SER	3.4
1	A	202	THR	3.3
2	B	164	GLY	3.3
2	B	134	THR	3.3
1	L	212	ASN	3.3
2	H	42	GLU	3.3
2	H	169	SER	3.3
2	B	43	LYS	3.3
2	H	195	SER	3.2
2	B	1	GLU	3.2
2	B	41	PRO	3.2
1	L	156	GLN	3.2
1	A	150	ILE	3.1
2	H	137	SER	3.1
2	H	179	GLN	3.1
2	B	136	SER	3.0
1	A	213	GLU	3.0
2	B	179	GLN	3.0
1	A	194[A]	CYS	3.0
1	A	201	SER	2.9
2	H	199	TRP	2.9
1	A	199	LYS	2.9
1	A	184[A]	ASP	2.9
2	H	193	VAL	2.9
2	H	168	SER	2.9
2	H	167	SER	2.8
1	L	152	GLY	2.8
2	B	169	SER	2.8
1	L	154	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	197	THR	2.7
1	A	200	THR	2.7
1	A	156	GLN	2.7
2	H	127	GLY	2.6
1	A	206	VAL	2.6
2	H	196	SER	2.6
1	L	135	PHE	2.5
2	H	222	LYS	2.5
1	L	209	PHE	2.5
1	A	159	VAL	2.4
1	L	145	ASN	2.4
2	B	135	GLY	2.4
1	A	205	ILE	2.4
1	L	203	SER	2.4
2	H	113[A]	SER	2.3
1	A	192	TYR	2.3
1	A	149	LYS	2.2
1	A	48	ILE	2.2
2	B	42	GLU	2.2
1	L	184[A]	ASP	2.1
2	H	200	PRO	2.1
2	B	195	SER	2.1
1	A	153	SER	2.1
2	H	205	VAL	2.1
1	A	32	TYR	2.0
1	L	199	LYS	2.0
1	L	200	THR	2.0
1	A	143	ASP	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,

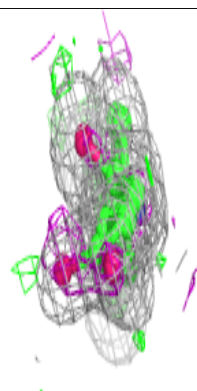
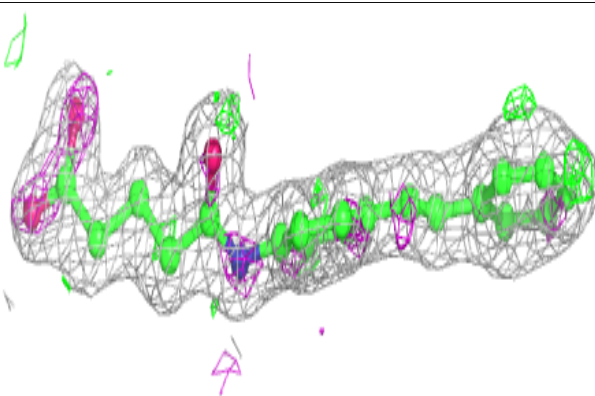
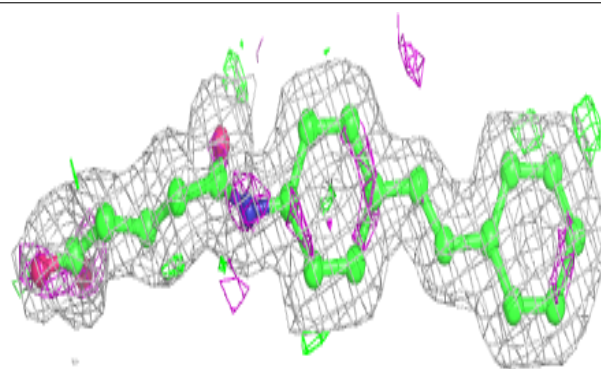
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

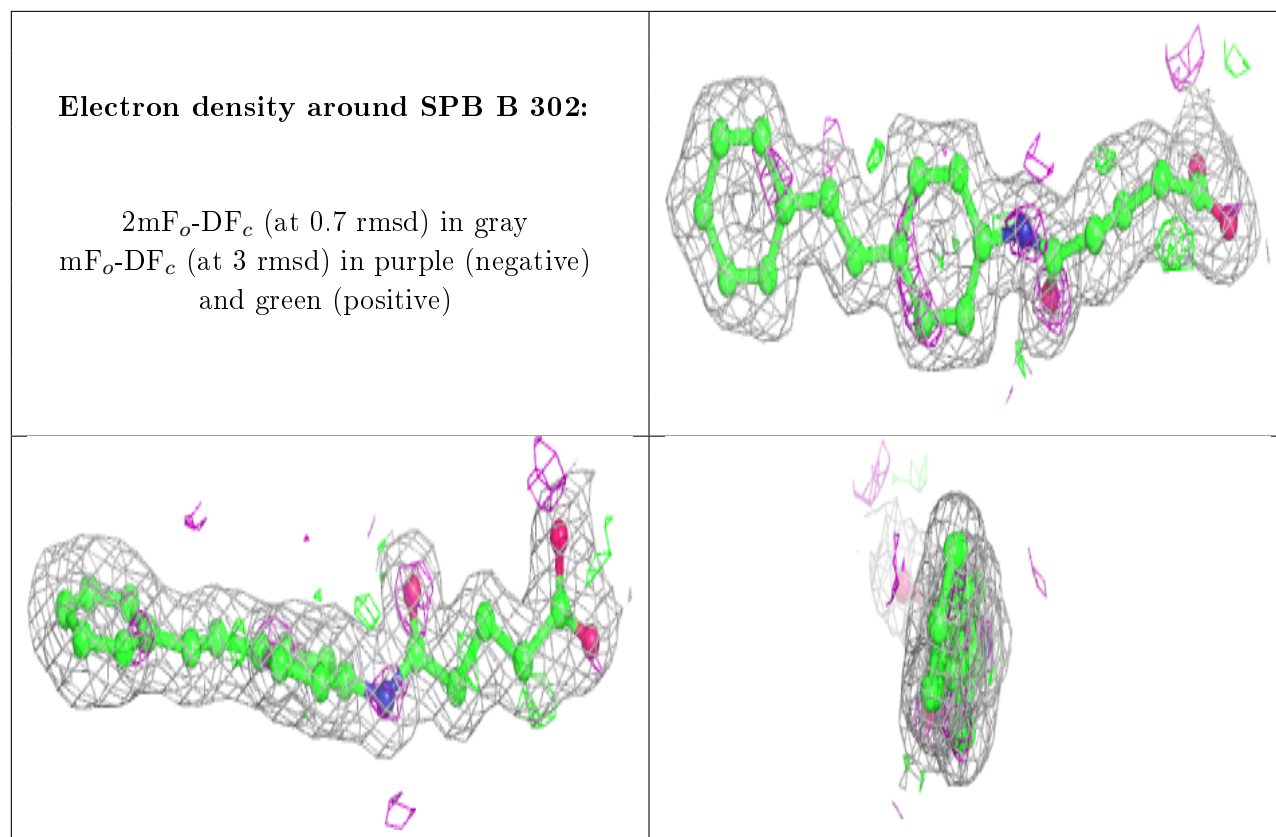
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	L	406	6/6	0.78	0.18	32,38,39,40	0
4	GOL	H	405	6/6	0.84	0.32	33,41,46,48	0
4	GOL	A	404	6/6	0.90	0.15	29,32,35,43	0
4	GOL	A	403	6/6	0.92	0.21	26,29,31,34	0
4	GOL	A	401	6/6	0.93	0.07	34,36,37,41	0
3	SPB	L	301	23/23	0.94	0.09	13,17,31,36	0
4	GOL	L	402	6/6	0.96	0.10	24,24,27,28	0
3	SPB	B	302	23/23	0.96	0.06	14,19,34,38	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 SPB L 301:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.