



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:46 PM UTC

PDB ID : 3CFB / pdb_00003cfb
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

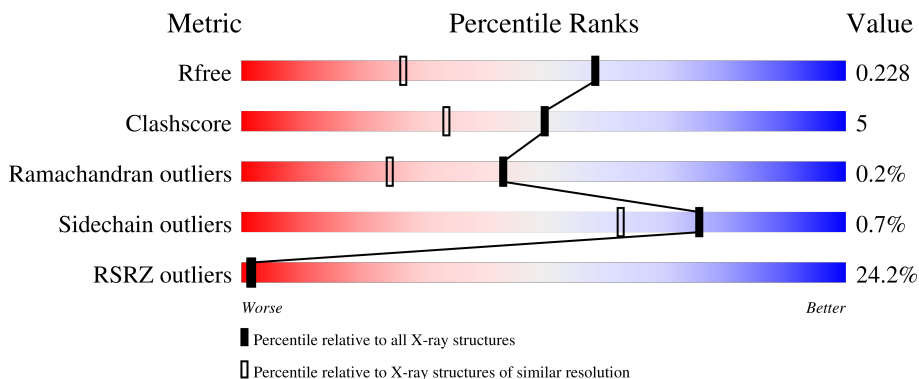
1 Overall quality at a glance

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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 of 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	219	
1	L	219	
2	B	213	
2	H	213	

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.

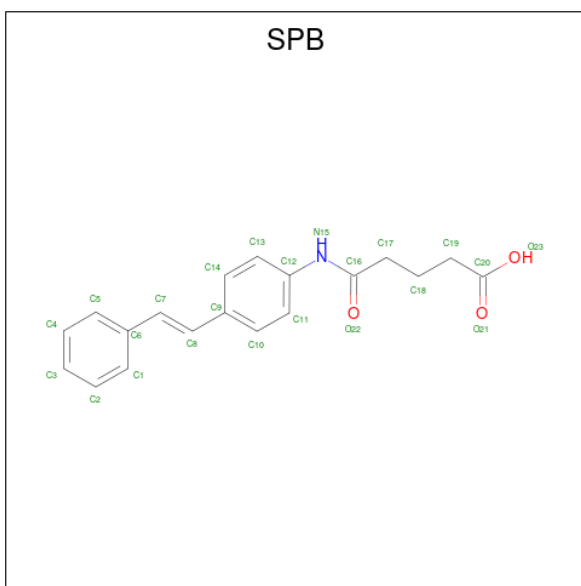
- Molecule 1 is a protein called BLUE FLUORESCENT ANTIBODY EP2-19G2-KAPPA LIGHT CHAIN.

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

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

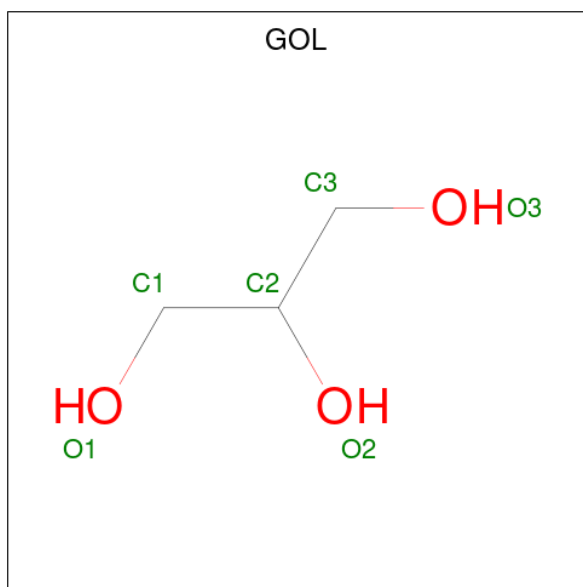
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	213	Total 1649	C 1036	N 275	O 329	S 9	0	8	0
2	B	213	Total 1628	C 1025	N 271	O 323	S 9	0	5	0

- Molecule 3 is 4-(4-STYRYL-PHENYL-CARBAMOYL)-BUTYRIC ACID (CCD ID: SPB) (formula: C₁₉H₁₉NO₃).



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 (CCD ID: GOL) (formula: C₃H₈O₃).



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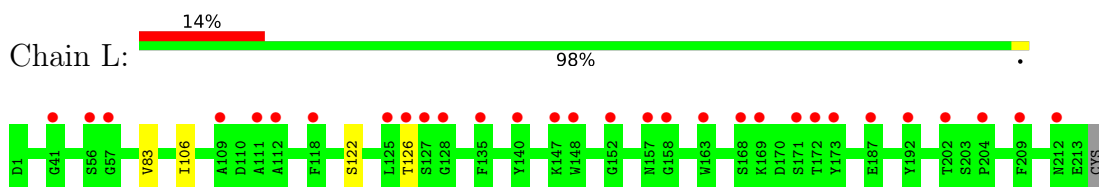
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	171	Total 171	O 171	0	0
5	B	124	Total 124	O 124	0	0

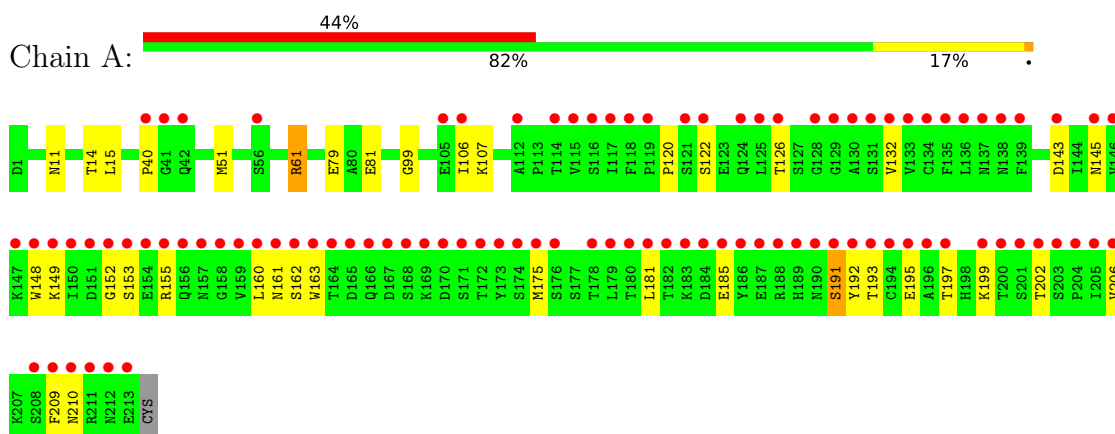
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

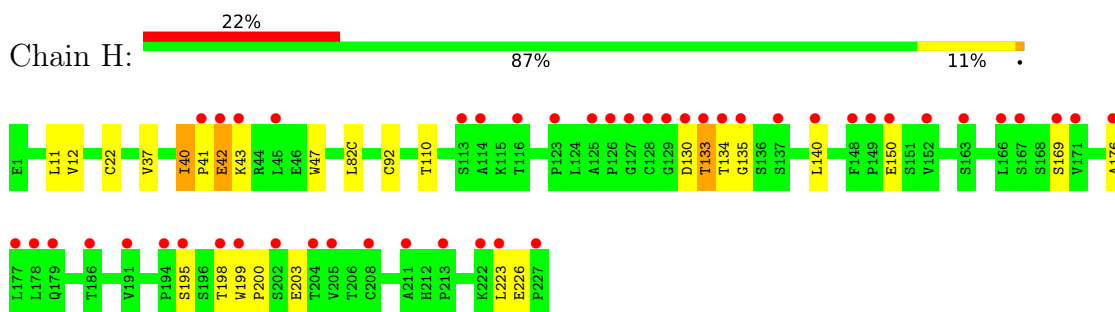
- Molecule 1: BLUE FLUORESCENT ANTIBODY EP2-19G2-KAPPA LIGHT CHAIN



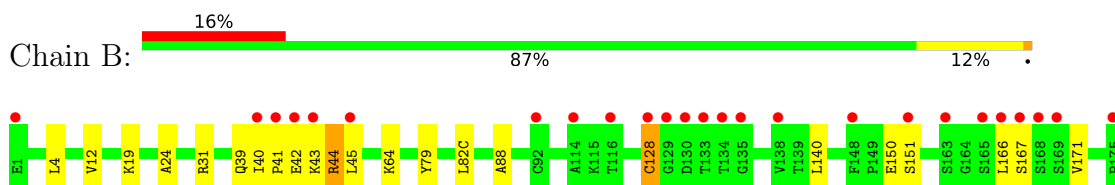
- Molecule 1: BLUE FLUORESCENT ANTIBODY EP2-19G2-KAPPA LIGHT CHAIN

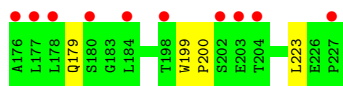


- Molecule 2: BLUE FLUORESCENT ANTIBODY EP2-19G2-IGG2B HEAVY CHAIN



- 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, α , β , γ	194.71Å 61.02Å 92.25Å 90.00° 116.65° 90.00°	Depositor
Resolution (Å)	42.03 – 1.60 42.03 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.03-1.60) 97.5 (42.03-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.60Å)	Xtrriage
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 (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtrriage
Anisotropy	0.199	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.009 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7457	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SPB, GOL

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	1.13	9/1800 (0.5%)	0.95	1/2445 (0.0%)
1	L	0.78	0/1782	0.82	0/2421
2	B	0.77	0/1667	0.86	0/2273
2	H	0.80	0/1688	0.81	0/2301
All	All	0.89	9/6937 (0.1%)	0.86	1/9440 (0.0%)

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	12.04	1.66	1.42
1	A	153	SER	C-O	11.41	1.37	1.24
1	A	192	TYR	C-O	9.50	1.36	1.24
1	A	210	ASN	CG-OD1	7.55	1.38	1.23
1	A	192	TYR	C-N	7.28	1.44	1.33
1	A	148	TRP	C-O	-6.79	1.15	1.24
1	A	61	ARG	CB-CG	-5.82	1.34	1.52
1	A	210	ASN	CG-ND2	5.70	1.45	1.33
1	A	148	TRP	CA-C	5.12	1.58	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ARG	CG-CD-NE	-6.77	97.11	112.00

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 [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	1763	0	1686	35	0
1	L	1745	0	1671	3	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:OG	1:A:191:SER:CB	1.66	1.42
1:A:51[A]:MET:HE1	5:A:571:HOH:O	1.36	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:149:LYS:C	5:A:537:HOH:O	2.40	0.64
1:A:14:THR:HG23	1:A:107:LYS:HE3	1.82	0.61
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:191:SER:CB	1:A:191:SER:HG	2.09	0.52
2:H:42:GLU:HG3	2:H:43:LYS:HG3	1.91	0.52
1:A:99:GLY:O	2:B:44:ARG:HG3	2.10	0.52
2:B:19:LYS:HE2	2:B:79:TYR:CD1	2.44	0.51
2:B:140:LEU:HB3	2:B:223:LEU:HD22	1.92	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
2:H:130:ASP:O	2:H:133:THR:CB	2.63	0.46
1:A:193:THR:CG2	1:A:206:VAL:HG13	2.46	0.46
2:H:22:CYS:SG	2:H:92[B]:CYS:CB	3.01	0.46
1:A:122:SER:O	1:A:126:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:161:ASN:HB3	1:A:175[A]: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
2:H:130:ASP:O	2:H:133:THR:HB	2.18	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: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
2:H:133:THR:CG2	2:H:134:THR:N	2.82	0.42
1:A:160:LEU:HD11	2:B:179:GLN:HG3	2.00	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:40:PRO:HG2	5:A:559:HOH:O	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: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%)	24	10
2	H	219/213 (103%)	212 (97%)	6 (3%)	1 (0%)	24	10
All	All	888/864 (103%)	863 (97%)	23 (3%)	2 (0%)	43	24

All (2) Ramachandran outliers are listed below:

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

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	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%)	81	70
2	H	192/184 (104%)	188 (98%)	4 (2%)	47	23
All	All	788/756 (104%)	783 (99%)	5 (1%)	76	66

All (5) 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	H	226	GLU
2	B	44	ARG

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

Mol	Chain	Res	Type
1	L	190	ASN
1	A	210	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	L	402	-	5,5,5	0.38	0	5,5,5	0.47	0
4	GOL	A	403	-	5,5,5	0.73	0	5,5,5	0.49	0
4	GOL	L	406	-	5,5,5	0.34	0	5,5,5	1.40	1 (20%)
3	SPB	L	301	-	24,24,24	0.74	0	30,30,30	1.19	2 (6%)
4	GOL	A	404	-	5,5,5	0.94	0	5,5,5	1.62	1 (20%)
4	GOL	H	405	-	5,5,5	0.27	0	5,5,5	0.80	0
4	GOL	A	401	-	5,5,5	0.58	0	5,5,5	0.72	0
3	SPB	B	302	-	24,24,24	0.84	0	30,30,30	1.12	2 (6%)

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	L	402	-	-	0/4/4/4	-
4	GOL	A	403	-	-	0/4/4/4	-
4	GOL	L	406	-	-	0/4/4/4	-
3	SPB	L	301	-	-	2/15/15/15	0/2/2/2
4	GOL	A	404	-	-	2/4/4/4	-
4	GOL	H	405	-	-	4/4/4/4	-
4	GOL	A	401	-	-	2/4/4/4	-
3	SPB	B	302	-	-	5/15/15/15	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	406	GOL	C3-C2-C1	-2.89	101.20	111.80
4	A	404	GOL	O3-C3-C2	-2.53	98.97	110.38
3	L	301	SPB	C19-C18-C17	-2.34	107.30	112.20
3	L	301	SPB	C18-C19-C20	-2.28	108.56	114.51
3	B	302	SPB	C3-C2-C1	-2.27	117.44	120.24
3	B	302	SPB	C13-C14-C9	2.24	124.11	121.22

There are no chirality outliers.

All (15) torsion outliers are listed below:

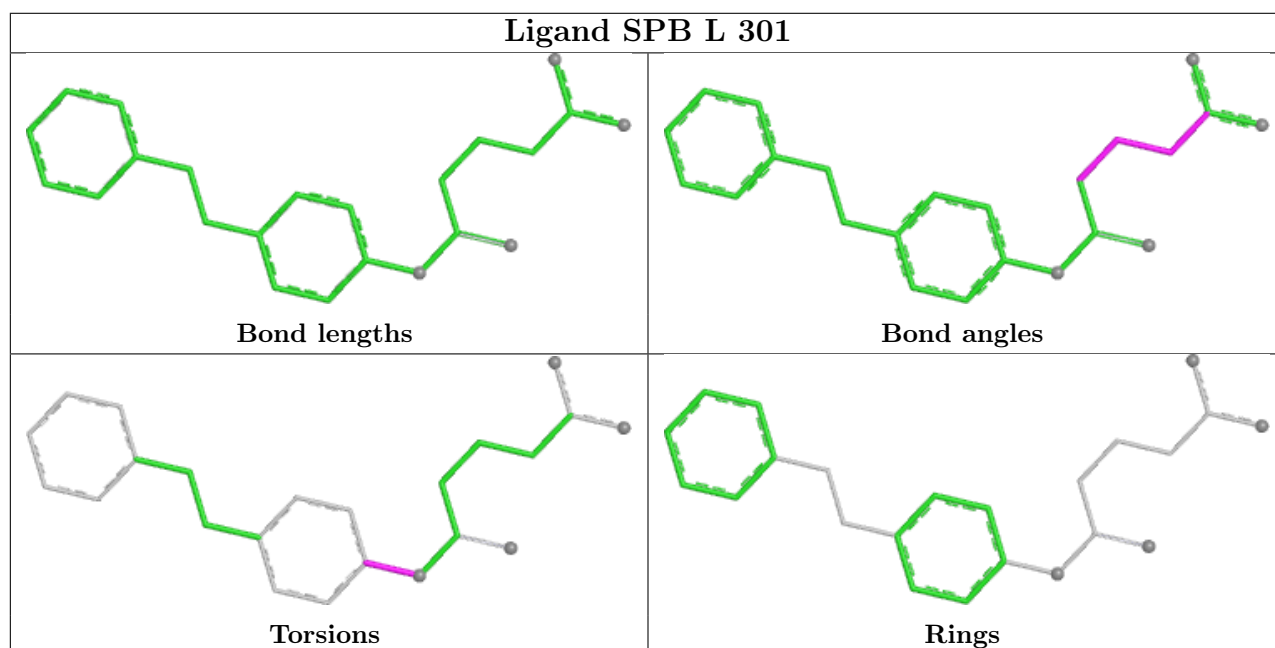
Mol	Chain	Res	Type	Atoms
4	H	405	GOL	C1-C2-C3-O3
4	A	404	GOL	O1-C1-C2-C3
4	A	401	GOL	O1-C1-C2-C3
4	H	405	GOL	O2-C2-C3-O3
4	A	404	GOL	O1-C1-C2-O2
3	B	302	SPB	C17-C18-C19-C20
4	A	401	GOL	O1-C1-C2-O2
3	L	301	SPB	C13-C12-N15-C16
4	H	405	GOL	O1-C1-C2-O2
4	H	405	GOL	O1-C1-C2-C3
3	B	302	SPB	C13-C12-N15-C16
3	B	302	SPB	C11-C12-N15-C16
3	B	302	SPB	C18-C19-C20-O21
3	L	301	SPB	C11-C12-N15-C16
3	B	302	SPB	C18-C19-C20-O23

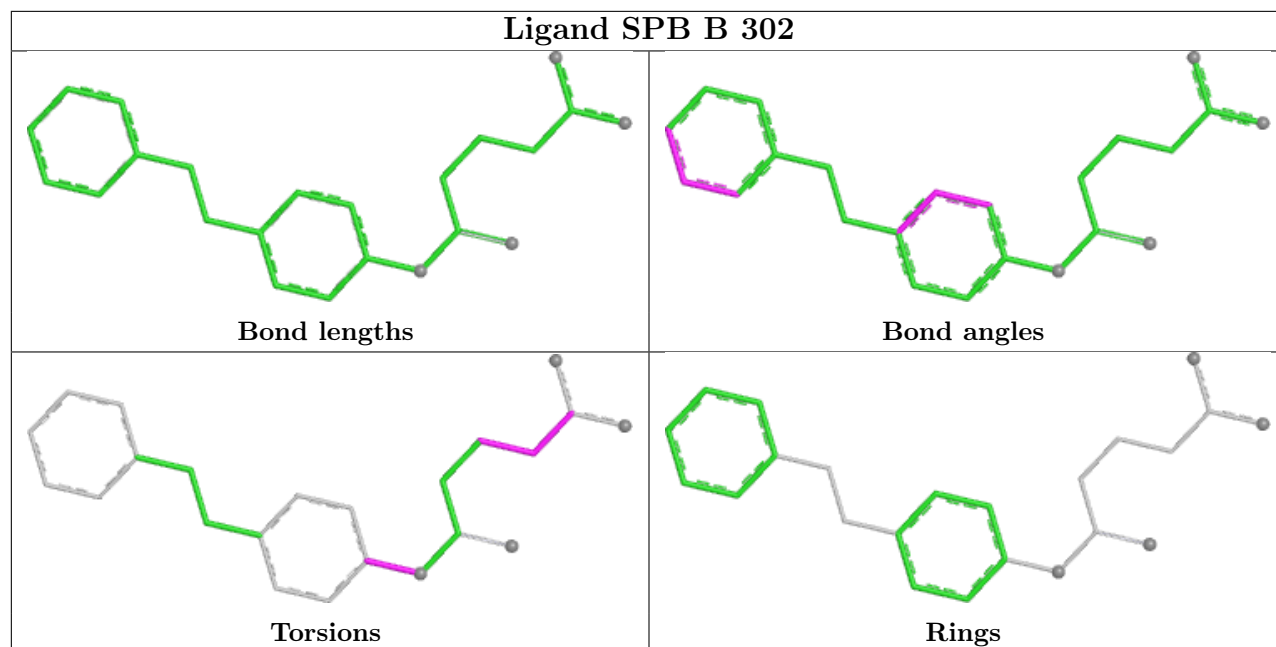
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	GOL	2	0
3	B	302	SPB	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, 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	218/219 (99%)	1.81	97 (44%) 0 0	7, 19, 27, 35	12 (5%)
1	L	218/219 (99%)	1.07	30 (13%) 6 6	9, 22, 29, 38	9 (4%)
2	B	213/213 (100%)	1.08	35 (16%) 4 4	8, 21, 31, 38	5 (2%)
2	H	213/213 (100%)	1.26	47 (22%) 2 2	9, 22, 32, 41	8 (3%)
All	All	862/864 (99%)	1.31	209 (24%) 2 1	7, 21, 30, 41	34 (3%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	128	CYS	7.3
2	H	133	THR	6.6
2	B	166	LEU	5.9
1	A	118	PHE	5.7
1	A	159	VAL	5.5
1	A	192	TYR	5.5
2	H	129	GLY	5.4
1	A	164	THR	5.4
2	B	130	ASP	5.3
1	A	194[A]	CYS	5.2
1	A	150	ILE	5.2
2	B	114	ALA	5.1
1	A	184[A]	ASP	5.1
1	A	132	VAL	5.0
1	A	206	VAL	4.9
1	A	124	GLN	4.8
1	A	126	THR	4.8
1	A	131	SER	4.7
1	A	205	ILE	4.7
2	H	130	ASP	4.7
1	A	181	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
2	H	137	SER	4.7
1	L	157	ASN	4.6
1	A	210	ASN	4.6
1	A	125	LEU	4.5
1	A	130	ALA	4.5
1	A	202	THR	4.5
2	H	127	GLY	4.4
2	H	128	CYS	4.4
1	A	135	PHE	4.3
1	A	201	SER	4.3
1	A	178	THR	4.3
1	A	147	LYS	4.3
1	A	148	TRP	4.3
2	H	125	ALA	4.3
1	A	133	VAL	4.3
1	A	151	ASP	4.2
1	A	186	TYR	4.2
1	A	197	THR	4.2
1	A	209	PHE	4.1
1	A	136	LEU	4.1
1	A	176	SER	4.0
1	A	213	GLU	4.0
1	A	153	SER	4.0
1	A	168[A]	SER	4.0
2	B	168	SER	4.0
1	L	109	ALA	4.0
1	A	160	LEU	3.9
1	A	146	VAL	3.9
1	A	162	SER	3.9
1	A	203	SER	3.8
2	H	194	PRO	3.8
1	A	129	GLY	3.8
2	H	42	GLU	3.8
1	A	191	SER	3.8
2	H	134	THR	3.7
1	A	167	ASP	3.7
1	A	121	SER	3.7
1	A	174	SER	3.7
1	A	163	TRP	3.7
1	A	143	ASP	3.7
1	A	172	THR	3.7
1	A	134	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	182	THR	3.6
1	A	128	GLY	3.6
2	B	129	GLY	3.6
1	A	179	LEU	3.6
2	B	184	LEU	3.5
1	A	119	PRO	3.5
1	A	204	PRO	3.5
1	A	169	LYS	3.4
2	B	227	PRO	3.4
1	A	154	GLU	3.4
1	A	200	THR	3.3
1	A	157	ASN	3.3
1	A	139	PHE	3.3
1	A	171	SER	3.3
1	A	145	ASN	3.3
2	H	114	ALA	3.3
1	A	41	GLY	3.2
2	H	135	GLY	3.2
1	A	122	SER	3.2
1	L	125	LEU	3.2
1	A	112	ALA	3.2
1	A	117	ILE	3.2
2	B	133	THR	3.2
1	A	156	GLN	3.1
2	B	43	LYS	3.1
1	L	168[A]	SER	3.1
2	H	179	GLN	3.1
2	H	227	PRO	3.1
1	A	138	ASN	3.1
2	B	45	LEU	3.1
1	A	152	GLY	3.0
1	A	42	GLN	3.0
1	A	199	LYS	3.0
1	A	193	THR	3.0
2	H	116	THR	3.0
1	A	175[A]	MET	3.0
1	A	115	VAL	3.0
1	L	212	ASN	3.0
1	A	187	GLU	3.0
1	A	180	THR	3.0
2	H	198	THR	3.0
2	B	163	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	177	LEU	3.0
2	B	204	THR	2.9
2	H	45	LEU	2.9
2	H	195	SER	2.9
2	B	167	SER	2.9
1	A	155	ARG	2.9
2	H	43	LYS	2.9
1	A	212	ASN	2.9
1	A	166	GLN	2.9
1	A	188	ARG	2.9
1	L	135	PHE	2.8
2	B	41	PRO	2.8
2	B	175	PRO	2.8
1	A	173	TYR	2.8
2	B	92[A]	CYS	2.8
2	B	134	THR	2.8
2	B	169	SER	2.8
1	A	137	ASN	2.7
1	A	165	ASP	2.7
2	B	135	GLY	2.7
2	H	223	LEU	2.7
2	B	165	SER	2.7
2	H	199	TRP	2.7
2	H	222	LYS	2.7
2	H	126	PRO	2.6
1	A	158	GLY	2.6
1	L	163	TRP	2.6
1	A	190	ASN	2.6
2	B	1	GLU	2.6
1	L	41	GLY	2.6
1	L	209	PHE	2.6
2	H	166	LEU	2.6
1	L	140	TYR	2.6
1	A	183	LYS	2.6
1	L	112	ALA	2.6
1	L	173	TYR	2.5
1	L	111	ALA	2.5
1	A	196	ALA	2.5
1	L	202	THR	2.5
1	A	189	HIS	2.5
2	H	202	SER	2.5
1	L	192	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	171	VAL	2.5
1	L	172	THR	2.5
1	L	127	SER	2.5
1	A	195	GLU	2.4
1	L	152	GLY	2.4
2	H	41	PRO	2.4
1	L	56	SER	2.4
1	L	147	LYS	2.4
2	H	148	PHE	2.4
1	A	106	ILE	2.4
2	B	203	GLU	2.4
1	L	204	PRO	2.4
2	H	140	LEU	2.4
1	L	148	TRP	2.4
1	A	161	ASN	2.3
1	A	185	GLU	2.3
1	A	211	ARG	2.3
2	B	116	THR	2.3
2	H	113[A]	SER	2.3
1	L	126	THR	2.3
2	B	178	LEU	2.3
2	B	138	VAL	2.3
1	L	128	GLY	2.3
2	H	177	LEU	2.3
2	B	148	PHE	2.3
2	H	204	THR	2.2
2	B	176	ALA	2.2
1	A	56[A]	SER	2.2
2	B	180	SER	2.2
1	L	118	PHE	2.2
2	H	152	VAL	2.2
2	H	123	PRO	2.2
1	L	158	GLY	2.2
2	B	40	ILE	2.2
2	H	186	THR	2.2
2	H	213	PRO	2.2
2	H	205	VAL	2.2
1	A	208	SER	2.2
2	H	167	SER	2.2
1	A	105	GLU	2.2
1	A	149	LYS	2.2
1	A	114	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	116	SER	2.2
2	H	163	SER	2.2
2	B	202	SER	2.2
1	L	187	GLU	2.1
2	B	42	GLU	2.1
1	L	169	LYS	2.1
2	H	149	PRO	2.1
2	B	198	THR	2.1
2	H	211	ALA	2.1
1	L	57	GLY	2.1
1	A	40	PRO	2.1
2	H	176	ALA	2.1
1	L	171	SER	2.1
2	B	151	SER	2.1
2	H	178	LEU	2.1
1	A	170	ASP	2.0
2	H	208	CYS	2.0
2	H	150	GLU	2.0
2	H	169	SER	2.0
2	H	191	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.

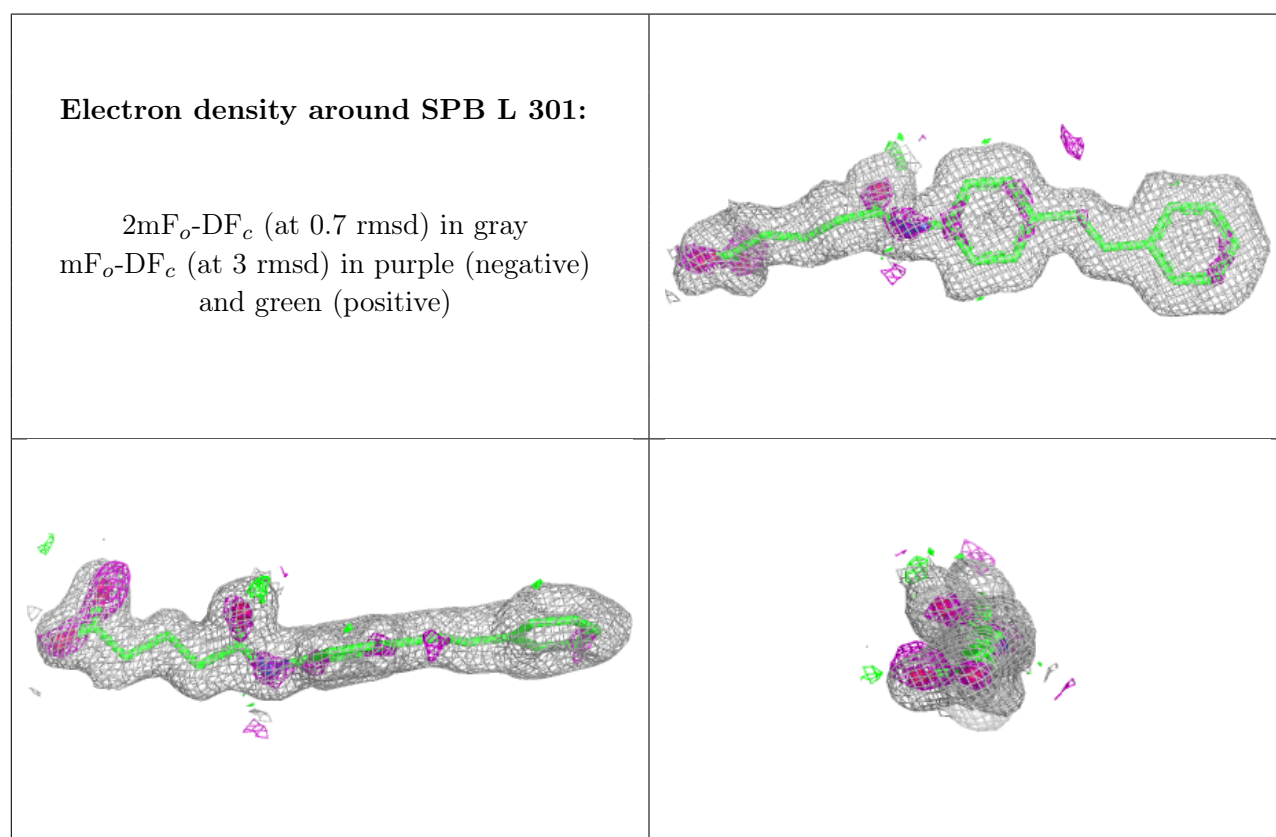
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	H	405	6/6	0.75	0.17	33,41,46,48	0
4	GOL	L	406	6/6	0.77	0.20	32,38,39,40	0
4	GOL	A	404	6/6	0.82	0.16	29,32,35,43	0

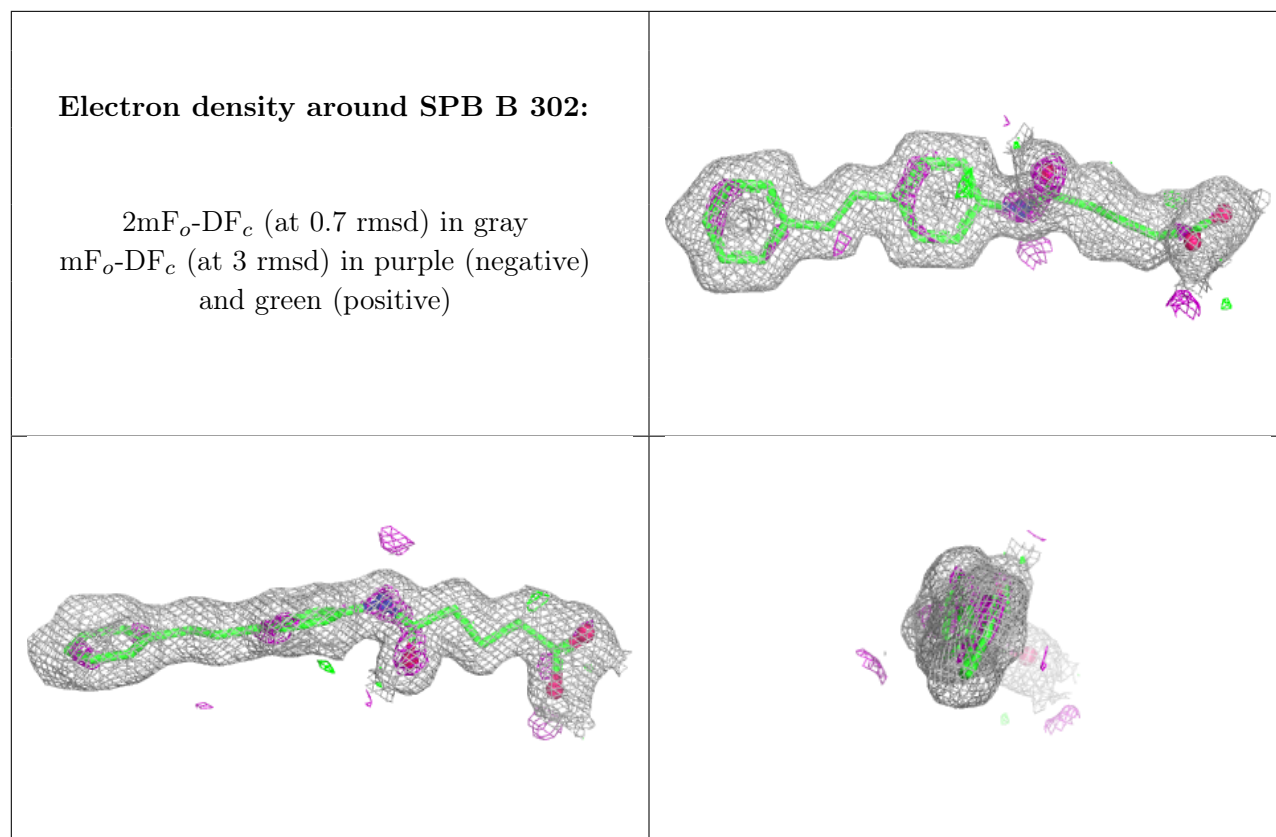
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	401	6/6	0.88	0.14	34,36,37,41	0
4	GOL	A	403	6/6	0.89	0.14	26,29,31,34	0
4	GOL	L	402	6/6	0.94	0.12	24,24,27,28	0
3	SPB	L	301	23/23	0.94	0.10	13,17,31,36	0
3	SPB	B	302	23/23	0.94	0.10	14,19,34,38	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.