



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:07 PM UTC

PDB ID : 9EBL / pdb\_00009eb1  
Title : Crystal structure of the hERbeta LBD complexed with androstenediol and SRC 2-2 peptide (crystal form 1)  
Authors : Pederick, J.L.; Bruning, J.B.  
Deposited on : 2024-11-12  
Resolution : 2.20 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.

The types of validation reports are described at

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

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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

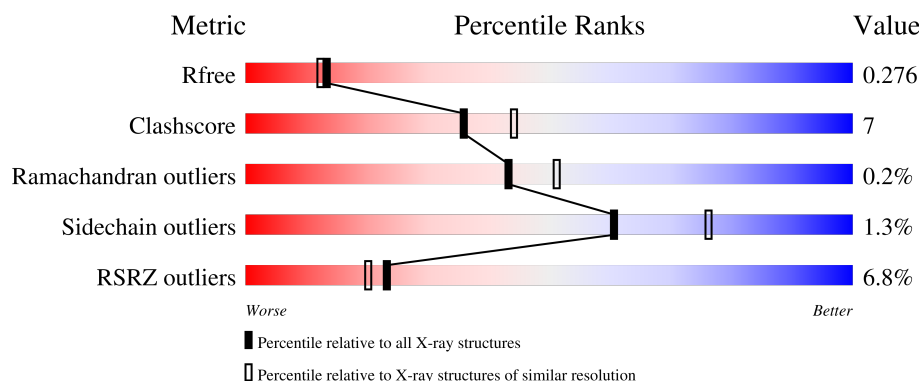
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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  $\geq 3$ , 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	239	<div> <div>10%</div> <div>78%</div> <div>14%</div> <div>8%</div> </div>
1	B	239	<div> <div>4%</div> <div>79%</div> <div>15%</div> <div>5%</div> </div>
1	E	239	<div> <div>8%</div> <div>73%</div> <div>18%</div> <div>8%</div> </div>
1	F	239	<div> <div>3%</div> <div>76%</div> <div>15%</div> <div>9%</div> </div>
2	C	13	<div> <div>46%</div> <div>8%</div> <div>46%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	13	 77%8%15%
2	G	13	 15%69%31%
2	H	13	 69%15%15%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7207 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.

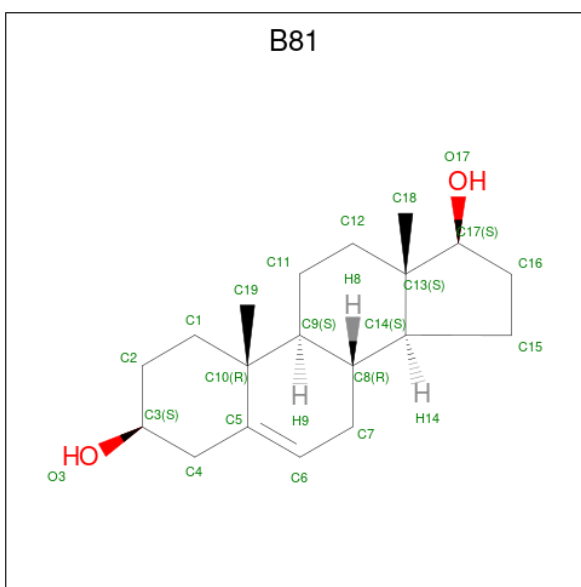
- Molecule 1 is a protein called Estrogen receptor beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1631	1044	278	290	19			
1	B	227	Total	C	N	O	S	0	0	0
			1774	1142	296	316	20			
1	E	219	Total	C	N	O	S	0	0	0
			1616	1033	272	292	19			
1	F	218	Total	C	N	O	S	0	0	0
			1683	1087	281	296	19			

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			47	30	10	7			
2	D	11	Total	C	N	O	0	0	0
			91	57	19	15			
2	G	9	Total	C	N	O	0	0	0
			68	43	14	11			
2	H	11	Total	C	N	O	0	0	0
			87	55	18	14			

- Molecule 3 is (3alpha,8alpha,17beta)-androst-5-ene-3,17-diol (CCD ID: B81) (formula: C<sub>19</sub>H<sub>30</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	19	2		
3	B	1	Total	C	O	0	0
			21	19	2		
3	E	1	Total	C	O	0	0
			21	19	2		
3	F	1	Total	C	O	0	0
			21	19	2		

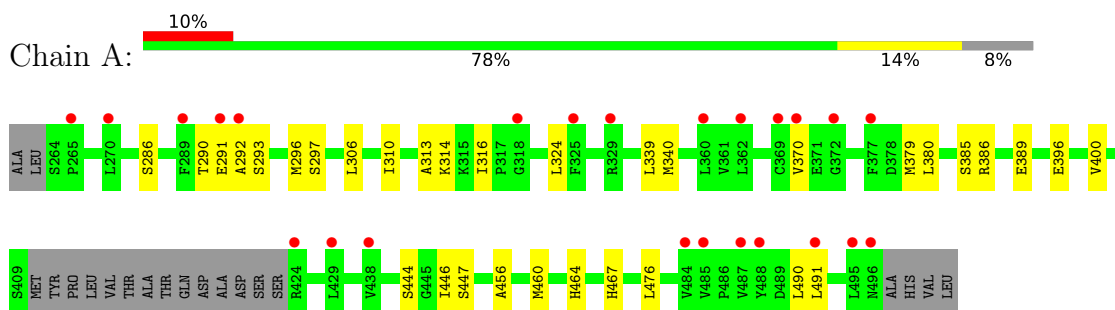
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	56	Total	O	0	0
			56	56		
4	D	3	Total	O	0	0
			3	3		
4	E	14	Total	O	0	0
			14	14		
4	F	45	Total	O	0	0
			45	45		

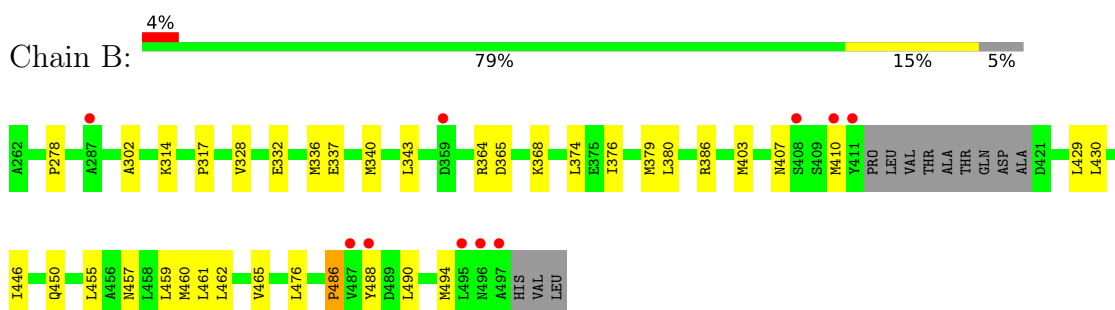
### 3 Residue-property plots

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.

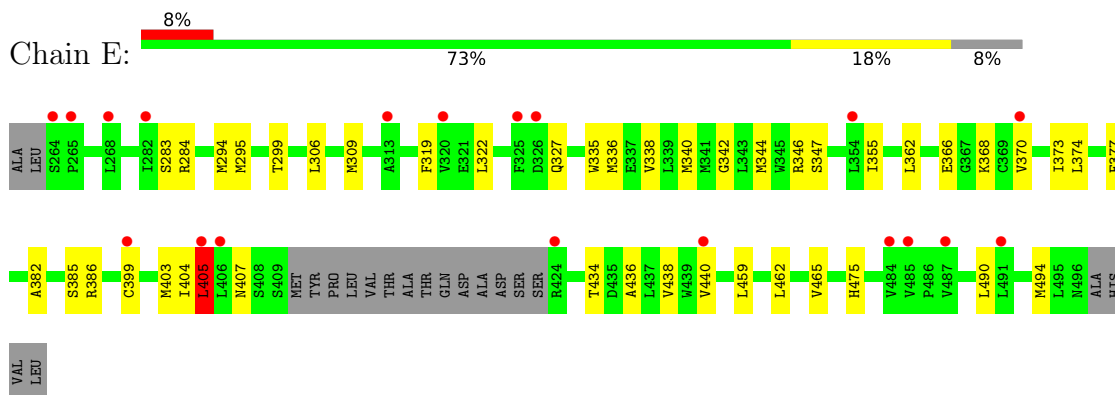
#### • Molecule 1: Estrogen receptor beta



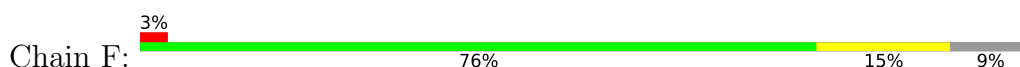
#### • Molecule 1: Estrogen receptor beta

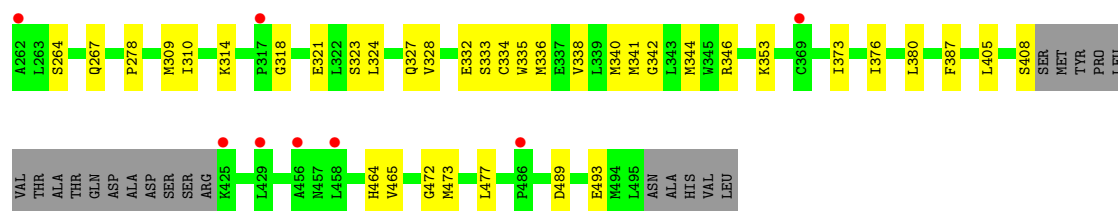


#### • Molecule 1: Estrogen receptor beta



#### • Molecule 1: Estrogen receptor beta

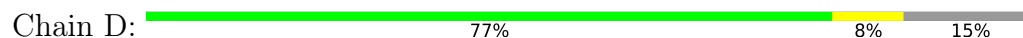




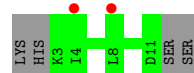
• Molecule 2: Nuclear receptor coactivator 2



• Molecule 2: Nuclear receptor coactivator 2



• Molecule 2: Nuclear receptor coactivator 2



• Molecule 2: Nuclear receptor coactivator 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.94Å 213.74Å 52.51Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	39.46 – 2.20 39.46 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.46-2.20) 93.0 (39.46-2.20)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.234 , 0.277 0.234 , 0.276	Depositor DCC
$R_{free}$ test set	2663 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B81

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	0.11	0/1658	0.29	0/2252
1	B	0.10	0/1806	0.26	0/2440
1	E	0.11	0/1642	0.30	0/2235
1	F	0.11	0/1713	0.26	0/2320
2	C	0.05	0/46	0.15	0/61
2	D	0.06	0/92	0.12	0/123
2	G	0.07	0/68	0.28	0/91
2	H	0.12	0/88	0.26	0/118
All	All	0.11	0/7113	0.27	0/9640

There are no bond length outliers.

There are no bond angle outliers.

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	1631	0	1616	24	0
1	B	1774	0	1832	26	0
1	E	1616	0	1582	31	0
1	F	1683	0	1739	28	0
2	C	47	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	91	0	89	1	0
2	G	68	0	62	0	0
2	H	87	0	83	4	0
3	A	21	0	30	1	0
3	B	21	0	30	3	0
3	E	21	0	30	1	0
3	F	21	0	30	1	0
4	A	8	0	0	0	0
4	B	56	0	0	1	0
4	D	3	0	0	0	0
4	E	14	0	0	0	0
4	F	45	0	0	2	0
All	All	7207	0	7165	104	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 7.

All (104) 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:E:373:ILE:HG13	1:E:475:HIS:CE1	2.12	0.84
1:A:310:ILE:HD11	1:A:490:LEU:HD21	1.69	0.74
1:E:370:VAL:HG11	1:E:373:ILE:HD12	1.73	0.71
1:E:284:ARG:NH2	1:E:366:GLU:OE1	2.23	0.70
1:B:376:ILE:HA	1:B:379:MET:HE3	1.76	0.68
1:A:290:THR:HG23	1:A:292:ALA:H	1.59	0.67
1:A:313:ALA:HA	1:A:316:ILE:HD12	1.77	0.66
1:F:344:MET:HE1	1:F:465:VAL:HG22	1.76	0.66
1:F:341:MET:HE3	1:F:344:MET:HE3	1.81	0.63
1:E:404:ILE:O	1:E:405:LEU:HB3	1.98	0.63
1:F:318:GLY:HA2	1:F:321:GLU:HG3	1.81	0.62
1:B:386:ARG:NH1	4:B:703:HOH:O	2.30	0.61
1:F:340:MET:HE2	1:F:380:LEU:HD21	1.83	0.61
1:F:332:GLU:OE2	2:H:2:HIS:NE2	2.27	0.61
1:B:317:PRO:O	1:B:429:LEU:HD21	2.02	0.59
1:B:337:GLU:HG2	1:B:465:VAL:HG12	1.85	0.58
1:E:344:MET:HE1	1:E:465:VAL:HG22	1.87	0.57
1:E:368:LYS:HA	1:E:374:LEU:HD11	1.85	0.57
1:B:340:MET:HG2	1:B:380:LEU:HD21	1.87	0.56
1:E:309:MET:HE2	1:E:338:VAL:HB	1.86	0.56
1:E:336:MET:SD	1:E:340:MET:HE3	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:VAL:O	1:B:332:GLU:HG3	2.07	0.55
1:A:314:LYS:HD2	2:C:9:LEU:HA	1.89	0.55
1:A:291:GLU:HA	1:A:370:VAL:HG22	1.88	0.55
1:F:336:MET:O	1:F:340:MET:HG3	2.08	0.54
1:E:370:VAL:CG1	1:E:373:ILE:HD12	2.36	0.54
1:B:386:ARG:HG2	1:B:461:LEU:HD21	1.91	0.53
1:E:399:CYS:O	1:E:403:MET:HG3	2.08	0.53
1:A:339:LEU:HB3	3:A:601:B81:H4A	1.92	0.52
1:F:328:VAL:O	1:F:332:GLU:HG3	2.09	0.52
1:F:376:ILE:HD13	1:F:472:GLY:HA2	1.92	0.52
1:F:473:MET:HG3	1:F:477:LEU:HD23	1.92	0.52
1:F:353:LYS:NZ	4:F:704:HOH:O	2.43	0.52
1:E:295:MET:O	1:E:299:THR:OG1	2.23	0.51
1:E:322:LEU:O	1:E:327:GLN:NE2	2.44	0.51
1:B:278:PRO:HB2	1:F:278:PRO:HB2	1.92	0.51
1:A:306:LEU:HB3	1:A:490:LEU:HD23	1.93	0.50
1:F:309:MET:HE2	1:F:338:VAL:HB	1.94	0.50
1:E:436:ALA:O	1:E:440:VAL:HG23	2.11	0.50
1:A:290:THR:H	1:A:293:SER:HG	1.59	0.49
1:A:460:MET:HG2	1:B:407:ASN:CG	2.37	0.49
1:A:385:SER:O	1:A:389:GLU:HG3	2.13	0.49
1:B:336:MET:SD	1:B:340:MET:HE3	2.53	0.48
1:E:370:VAL:HG11	1:E:373:ILE:CD1	2.42	0.48
1:B:446:ILE:HD12	1:B:450:GLN:HB3	1.94	0.48
1:F:340:MET:O	1:F:344:MET:HG3	2.12	0.48
1:E:319:PHE:HE1	1:E:405:LEU:HD11	1.77	0.48
1:E:373:ILE:HG12	3:E:601:B81:H16	1.95	0.48
1:E:373:ILE:HG23	1:E:377:PHE:CE1	2.49	0.47
1:A:476:LEU:HD21	1:A:491:LEU:HD11	1.97	0.47
1:B:314:LYS:HD2	2:D:9:LEU:HA	1.95	0.47
1:A:306:LEU:O	1:A:310:ILE:HG13	2.15	0.47
1:F:341:MET:HE1	1:F:387:PHE:CE2	2.50	0.46
1:A:290:THR:HG22	1:A:293:SER:H	1.80	0.46
1:B:364:ARG:CZ	1:B:374:LEU:HD11	2.45	0.46
1:B:302:ALA:HB2	3:B:601:B81:H1	1.98	0.46
1:F:336:MET:HE2	1:F:473:MET:HE2	1.98	0.46
1:B:476:LEU:HB2	3:B:601:B81:H18B	1.98	0.45
1:E:319:PHE:CE2	1:E:327:GLN:HG2	2.51	0.45
1:E:306:LEU:HD21	1:E:335:TRP:CE3	2.51	0.45
1:F:323:SER:O	1:F:327:GLN:HG3	2.17	0.45
1:F:493:GLU:OE2	2:H:2:HIS:ND1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:GLY:O	1:F:346:ARG:HG3	2.16	0.45
1:F:473:MET:HE2	1:F:473:MET:HB2	1.76	0.45
1:F:264:SER:N	1:F:267:GLN:OE1	2.41	0.44
1:F:373:ILE:HG13	3:F:601:B81:H16	1.99	0.44
1:E:382:ALA:O	1:E:386:ARG:HG2	2.17	0.44
1:E:347:SER:HG	1:E:355:ILE:H	1.63	0.44
1:B:457:ASN:HA	1:B:460:MET:HE3	1.99	0.44
1:E:407:ASN:ND2	1:F:464:HIS:HE1	2.16	0.43
1:B:403:MET:HE1	1:B:459:LEU:HD22	2.00	0.43
1:F:314:LYS:NZ	2:H:8:LEU:O	2.50	0.43
1:A:340:MET:HE2	1:A:380:LEU:HD21	2.01	0.43
1:A:464:HIS:CD2	1:B:410:MET:HG3	2.54	0.43
1:B:455:LEU:O	1:B:459:LEU:HG	2.18	0.43
1:A:379:MET:HE1	1:A:467:HIS:CD2	2.54	0.43
1:A:444:SER:HB3	1:A:446:ILE:HG13	1.99	0.43
1:B:486:PRO:HB2	1:B:488:TYR:CE2	2.54	0.43
1:B:429:LEU:HA	1:B:429:LEU:HD23	1.81	0.43
1:A:464:HIS:NE2	1:B:410:MET:HG3	2.34	0.43
1:F:334:CYS:SG	1:F:405:LEU:HD23	2.59	0.43
1:A:340:MET:HG2	1:A:380:LEU:HD21	2.01	0.42
1:E:374:LEU:H	1:E:374:LEU:HD12	1.84	0.42
1:E:295:MET:SD	1:E:373:ILE:HD11	2.59	0.42
1:E:336:MET:HE2	1:E:336:MET:HB2	1.83	0.42
1:B:459:LEU:HA	1:B:462:LEU:HD23	2.02	0.42
1:A:386:ARG:HA	1:A:386:ARG:HD2	1.59	0.42
1:E:294:MET:HE2	1:E:362:LEU:HD13	2.00	0.42
1:E:434:THR:O	1:E:438:VAL:HG23	2.19	0.42
1:A:446:ILE:HG22	1:A:447:SER:H	1.85	0.42
1:F:309:MET:HE1	1:F:335:TRP:O	2.20	0.41
1:B:365:ASP:O	1:B:368:LYS:HG3	2.20	0.41
1:E:490:LEU:O	1:E:494:MET:HG2	2.20	0.41
1:A:456:ALA:O	1:A:460:MET:HB2	2.20	0.41
1:B:343:LEU:HD22	3:B:601:B81:H6	2.03	0.41
1:E:459:LEU:HD22	1:E:462:LEU:HD11	2.03	0.41
1:E:370:VAL:CB	1:E:373:ILE:HD12	2.50	0.41
1:F:310:ILE:HG21	2:H:8:LEU:HB3	2.02	0.41
1:F:324:LEU:O	1:F:328:VAL:HG23	2.21	0.40
1:A:396:GLU:O	1:A:400:VAL:HG23	2.20	0.40
1:B:490:LEU:O	1:B:494:MET:HG2	2.22	0.40
1:A:379:MET:HE2	1:A:379:MET:HB3	1.79	0.40
1:E:342:GLY:O	1:E:346:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:489:ASP:N	4:F:706:HOH:O	2.49	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	215/239 (90%)	205 (95%)	10 (5%)	0	100	100
1	B	223/239 (93%)	217 (97%)	5 (2%)	1 (0%)	30	34
1	E	215/239 (90%)	207 (96%)	7 (3%)	1 (0%)	24	27
1	F	214/239 (90%)	208 (97%)	6 (3%)	0	100	100
2	C	5/13 (38%)	5 (100%)	0	0	100	100
2	D	9/13 (69%)	8 (89%)	1 (11%)	0	100	100
2	G	7/13 (54%)	7 (100%)	0	0	100	100
2	H	9/13 (69%)	8 (89%)	1 (11%)	0	100	100
All	All	897/1008 (89%)	865 (96%)	30 (3%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	405	LEU
1	B	486	PRO

### 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	171/214 (80%)	167 (98%)	4 (2%)	44	59
1	B	199/214 (93%)	198 (100%)	1 (0%)	81	90
1	E	169/214 (79%)	166 (98%)	3 (2%)	51	68
1	F	187/214 (87%)	185 (99%)	2 (1%)	65	79
2	C	3/13 (23%)	3 (100%)	0	100	100
2	D	10/13 (77%)	10 (100%)	0	100	100
2	G	6/13 (46%)	6 (100%)	0	100	100
2	H	9/13 (69%)	9 (100%)	0	100	100
All	All	754/908 (83%)	744 (99%)	10 (1%)	61	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	SER
1	A	296	MET
1	A	297	SER
1	A	324	LEU
1	B	430	LEU
1	E	283	SER
1	E	385	SER
1	E	405	LEU
1	F	333	SER
1	F	408	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	GLN
1	A	483	ASN
1	B	431	ASN
1	E	327	GLN
1	E	350	HIS
1	E	407	ASN
1	E	457	ASN
1	F	464	HIS

### 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](#)

4 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$
3	B81	B	601	-	24,24,24	1.71	6 (25%)	39,39,39	2.50	15 (38%)
3	B81	A	601	-	24,24,24	1.83	7 (29%)	39,39,39	2.59	15 (38%)
3	B81	F	601	-	24,24,24	1.84	6 (25%)	39,39,39	2.58	14 (35%)
3	B81	E	601	-	24,24,24	1.82	7 (29%)	39,39,39	2.58	15 (38%)

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
3	B81	B	601	-	-	-	0/4/4/4
3	B81	A	601	-	-	-	0/4/4/4
3	B81	F	601	-	-	-	0/4/4/4
3	B81	E	601	-	-	-	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	601	B81	C10-C9	4.93	1.63	1.56
3	E	601	B81	C10-C9	4.91	1.63	1.56
3	A	601	B81	C10-C9	4.72	1.63	1.56
3	B	601	B81	C10-C9	4.31	1.62	1.56
3	F	601	B81	C8-C14	3.29	1.59	1.53
3	E	601	B81	C8-C14	3.26	1.59	1.53
3	A	601	B81	C8-C14	3.21	1.59	1.53
3	A	601	B81	C7-C8	3.03	1.58	1.53
3	B	601	B81	C8-C14	2.94	1.59	1.53
3	B	601	B81	C7-C8	2.93	1.57	1.53
3	F	601	B81	C7-C8	2.74	1.57	1.53
3	E	601	B81	C7-C8	2.66	1.57	1.53
3	F	601	B81	C4-C3	2.32	1.56	1.52
3	F	601	B81	C11-C9	2.30	1.57	1.53
3	B	601	B81	C11-C9	2.29	1.57	1.53
3	A	601	B81	C11-C9	2.21	1.57	1.53
3	E	601	B81	C4-C3	2.18	1.56	1.52
3	E	601	B81	C11-C9	2.18	1.57	1.53
3	B	601	B81	C4-C5	2.14	1.56	1.51
3	F	601	B81	C4-C5	2.11	1.55	1.51
3	A	601	B81	C4-C5	2.10	1.55	1.51
3	B	601	B81	C4-C3	2.10	1.55	1.52
3	E	601	B81	O17-C17	-2.07	1.40	1.43
3	A	601	B81	C13-C17	2.07	1.57	1.54
3	E	601	B81	C4-C5	2.03	1.55	1.51
3	A	601	B81	C12-C11	2.02	1.57	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	601	B81	C14-C13-C17	6.78	106.16	99.25
3	A	601	B81	C14-C13-C17	6.63	106.01	99.25
3	E	601	B81	C14-C13-C17	6.45	105.82	99.25
3	E	601	B81	C4-C5-C6	5.98	128.67	120.57
3	F	601	B81	C4-C5-C6	5.81	128.45	120.57
3	B	601	B81	C14-C13-C17	5.80	105.16	99.25
3	A	601	B81	C4-C5-C6	5.73	128.34	120.57
3	B	601	B81	C4-C5-C6	5.53	128.06	120.57
3	A	601	B81	C18-C13-C12	-5.28	102.83	110.61
3	E	601	B81	C18-C13-C12	-5.23	102.89	110.61
3	A	601	B81	C7-C8-C14	5.17	118.25	110.93
3	E	601	B81	C15-C14-C13	-5.17	97.76	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	601	B81	C18-C13-C12	-5.17	102.99	110.61
3	B	601	B81	C15-C14-C13	-5.12	97.81	103.84
3	A	601	B81	C15-C14-C13	-5.05	97.90	103.84
3	F	601	B81	C15-C14-C13	-4.97	97.99	103.84
3	E	601	B81	C7-C8-C14	4.95	117.94	110.93
3	F	601	B81	C7-C8-C14	4.94	117.93	110.93
3	B	601	B81	C18-C13-C12	-4.93	103.33	110.61
3	B	601	B81	C7-C8-C14	4.47	117.27	110.93
3	F	601	B81	C9-C10-C5	3.96	115.44	109.65
3	E	601	B81	C9-C10-C5	3.94	115.42	109.65
3	A	601	B81	C9-C10-C5	3.61	114.94	109.65
3	A	601	B81	C12-C11-C9	3.43	118.96	113.14
3	E	601	B81	C12-C11-C9	3.31	118.76	113.14
3	F	601	B81	C12-C11-C9	3.27	118.70	113.14
3	A	601	B81	C7-C8-C9	-3.27	105.94	109.72
3	B	601	B81	C12-C11-C9	3.16	118.51	113.14
3	B	601	B81	C9-C10-C5	3.15	114.27	109.65
3	B	601	B81	C10-C5-C6	-3.09	118.42	122.93
3	E	601	B81	C4-C5-C10	-3.03	112.54	116.42
3	F	601	B81	O17-C17-C13	-2.97	108.58	114.80
3	B	601	B81	C7-C8-C9	-2.96	106.30	109.72
3	B	601	B81	O17-C17-C13	-2.95	108.62	114.80
3	E	601	B81	O17-C17-C13	-2.94	108.65	114.80
3	F	601	B81	C4-C5-C10	-2.93	112.66	116.42
3	A	601	B81	C10-C5-C6	-2.85	118.77	122.93
3	B	601	B81	C8-C7-C6	2.85	116.71	112.76
3	E	601	B81	C10-C5-C6	-2.84	118.79	122.93
3	A	601	B81	O17-C17-C13	-2.82	108.90	114.80
3	F	601	B81	C10-C5-C6	-2.77	118.89	122.93
3	A	601	B81	C11-C12-C13	-2.76	108.09	112.74
3	A	601	B81	C4-C5-C10	-2.76	112.89	116.42
3	E	601	B81	C7-C8-C9	-2.75	106.54	109.72
3	F	601	B81	C7-C8-C9	-2.62	106.69	109.72
3	B	601	B81	C1-C10-C9	-2.62	105.27	108.74
3	B	601	B81	C11-C12-C13	-2.61	108.33	112.74
3	F	601	B81	C11-C12-C13	-2.59	108.36	112.74
3	B	601	B81	C16-C17-C13	-2.59	102.48	104.52
3	E	601	B81	C11-C12-C13	-2.44	108.62	112.74
3	B	601	B81	C4-C5-C10	-2.27	113.52	116.42
3	F	601	B81	C8-C7-C6	2.19	115.80	112.76
3	E	601	B81	C8-C7-C6	2.17	115.77	112.76
3	E	601	B81	C1-C10-C9	-2.17	105.87	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	601	B81	C1-C10-C9	-2.14	105.90	108.74
3	A	601	B81	C1-C10-C9	-2.12	105.93	108.74
3	A	601	B81	C8-C7-C6	2.09	115.66	112.76
3	A	601	B81	C3-C4-C5	2.05	115.31	112.05
3	E	601	B81	C2-C1-C10	2.02	117.09	112.78

There are no chirality outliers.

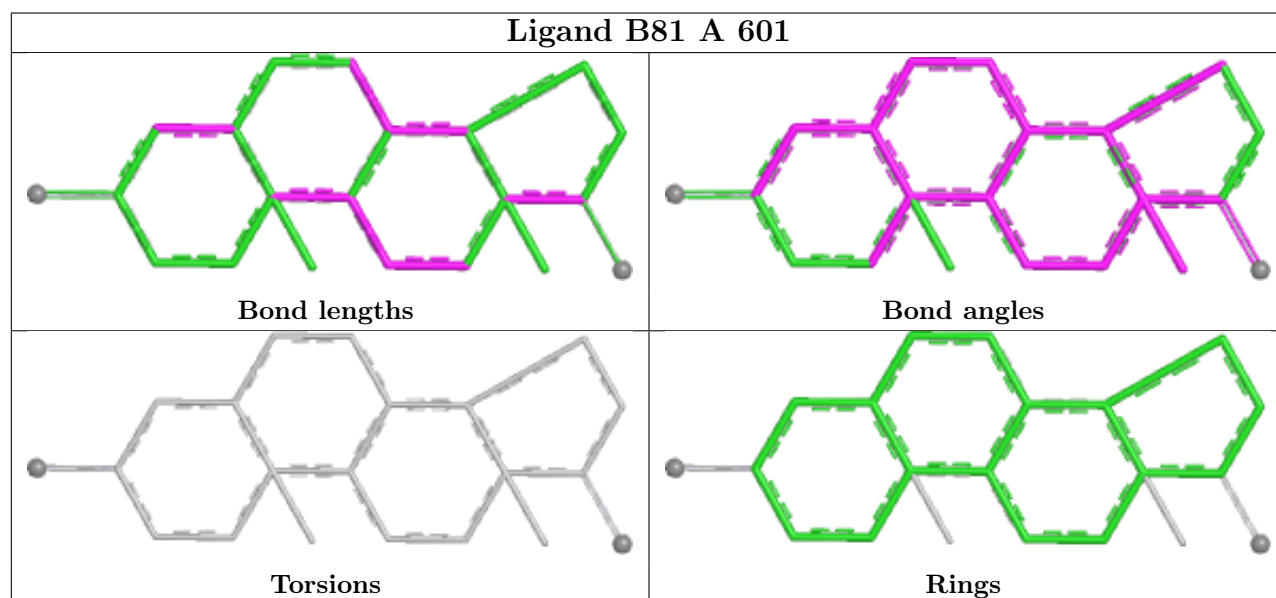
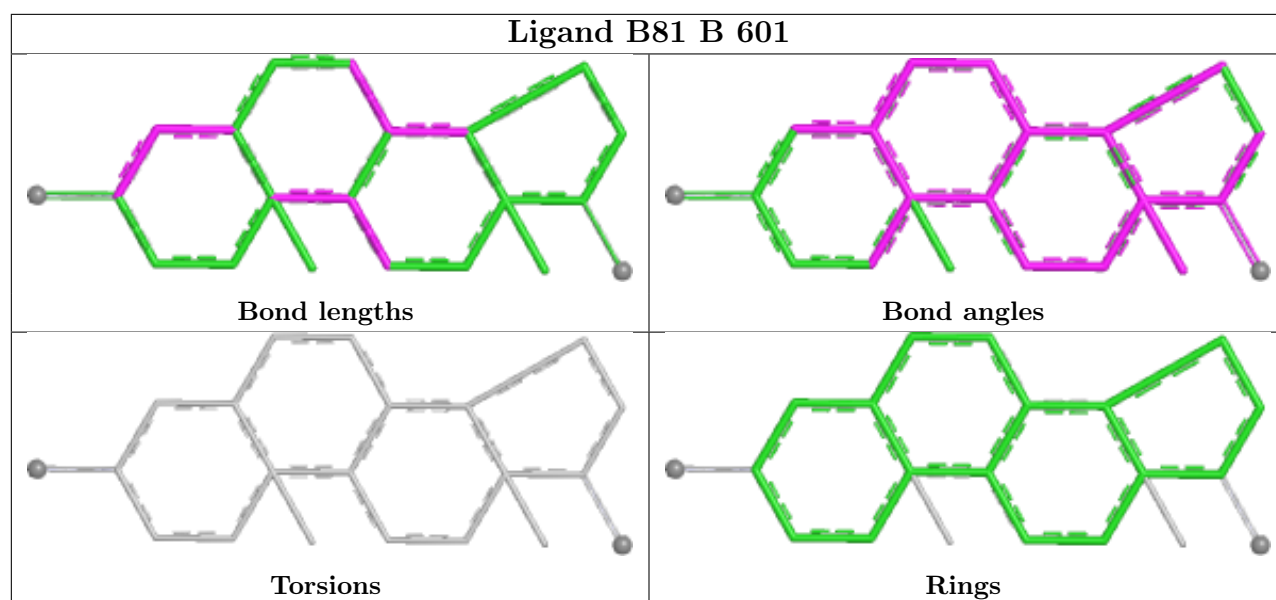
There are no torsion outliers.

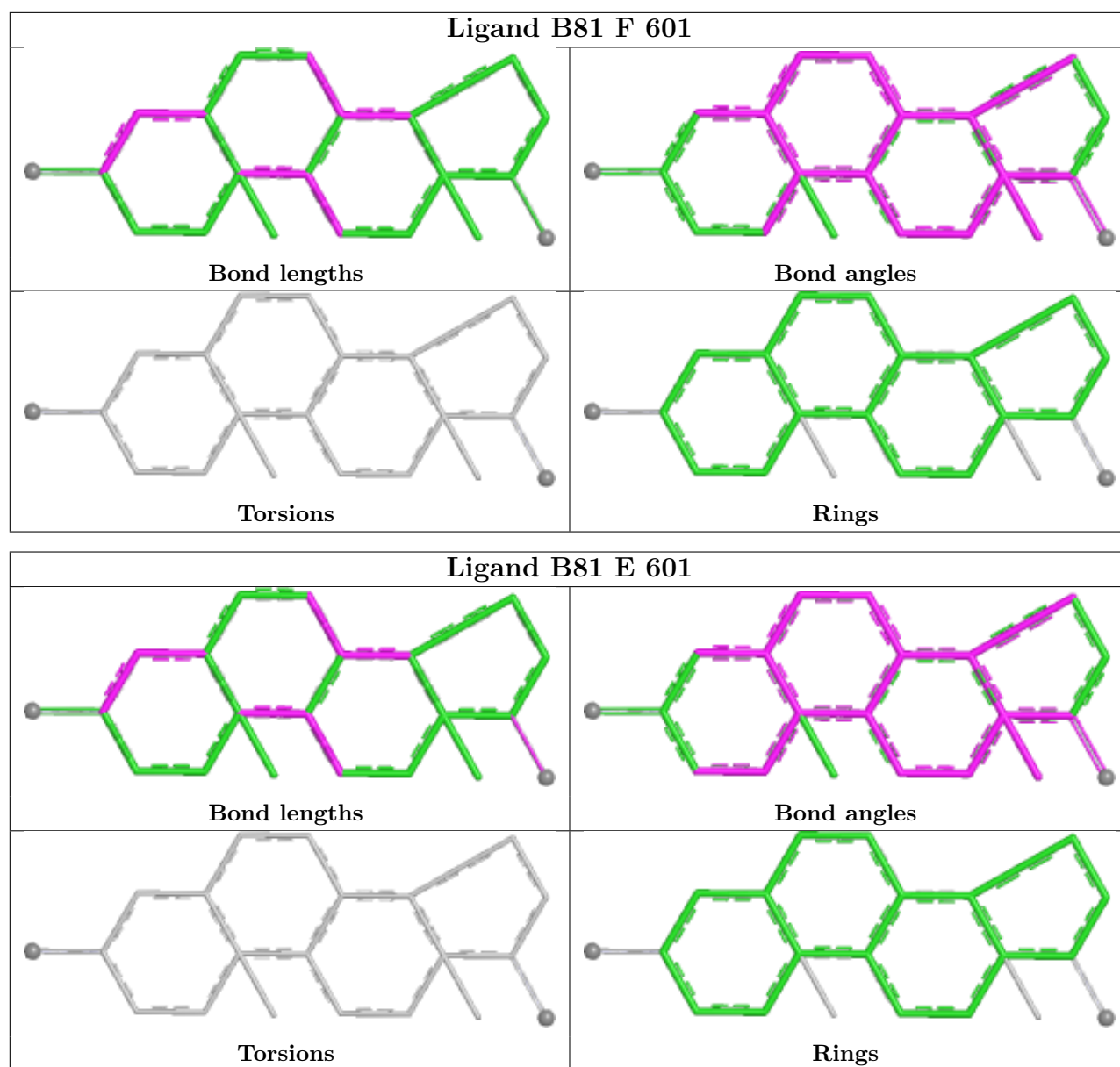
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	B81	3	0
3	A	601	B81	1	0
3	F	601	B81	1	0
3	E	601	B81	1	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	219/239 (91%)	0.91	24 (10%) 10 8	38, 66, 108, 131	0
1	B	227/239 (94%)	0.36	10 (4%) 39 36	23, 39, 66, 110	0
1	E	219/239 (91%)	0.93	19 (8%) 16 13	46, 65, 94, 119	0
1	F	218/239 (91%)	0.43	8 (3%) 45 42	31, 49, 71, 96	0
2	C	7/13 (53%)	0.87	0 100 100	69, 72, 75, 78	0
2	D	11/13 (84%)	0.36	0 100 100	43, 48, 70, 71	0
2	G	9/13 (69%)	1.87	2 (22%) 2 1	84, 91, 114, 121	0
2	H	11/13 (84%)	0.57	0 100 100	50, 60, 73, 79	0
All	All	921/1008 (91%)	0.66	63 (6%) 23 20	23, 56, 94, 131	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	487	VAL	4.8
1	B	497	ALA	4.0
2	G	4	ILE	3.6
1	E	313	ALA	3.5
1	E	325	PHE	3.5
1	A	289	PHE	3.3
1	E	399	CYS	3.1
1	B	496	ASN	3.1
1	A	485	VAL	3.1
1	E	406	LEU	3.1
1	A	495	LEU	3.0
1	B	411	TYR	3.0
1	A	292	ALA	2.9
1	E	320	VAL	2.8
1	B	410	MET	2.8
1	F	429	LEU	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	491	LEU	2.6
1	A	291	GLU	2.6
1	A	318	GLY	2.6
1	A	265	PRO	2.6
1	E	268	LEU	2.5
1	B	287	ALA	2.5
1	F	456	ALA	2.5
1	A	329	ARG	2.5
1	A	487	VAL	2.5
1	F	458	LEU	2.5
1	A	372	GLY	2.5
1	E	405	LEU	2.4
1	F	486	PRO	2.4
1	A	370	VAL	2.4
1	A	438	VAL	2.4
1	E	326	ASP	2.4
1	E	424	ARG	2.4
1	A	488	TYR	2.3
1	E	264	SER	2.3
1	A	369	CYS	2.3
1	E	265	PRO	2.3
1	A	484	VAL	2.3
1	A	429	LEU	2.3
1	E	485	VAL	2.3
1	A	377	PHE	2.2
1	B	487	VAL	2.2
1	B	495	LEU	2.2
2	G	8	LEU	2.2
1	A	496	ASN	2.2
1	F	262	ALA	2.2
1	E	282	ILE	2.1
1	F	317	PRO	2.1
1	B	408	SER	2.1
1	A	270	LEU	2.1
1	A	491	LEU	2.1
1	A	325	PHE	2.1
1	A	424	ARG	2.1
1	A	362	LEU	2.1
1	E	354	LEU	2.1
1	E	370	VAL	2.1
1	F	425	LYS	2.1
1	F	369	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	359	ASP	2.0
1	B	488	TYR	2.0
1	E	440	VAL	2.0
1	E	484	VAL	2.0
1	A	360	LEU	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, 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.

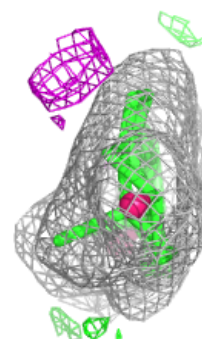
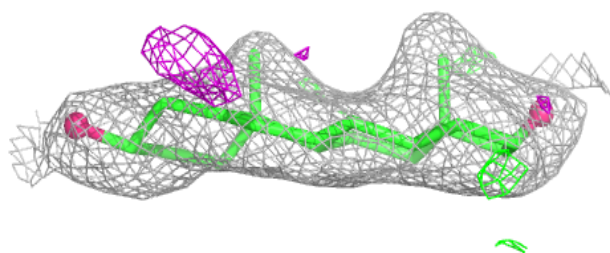
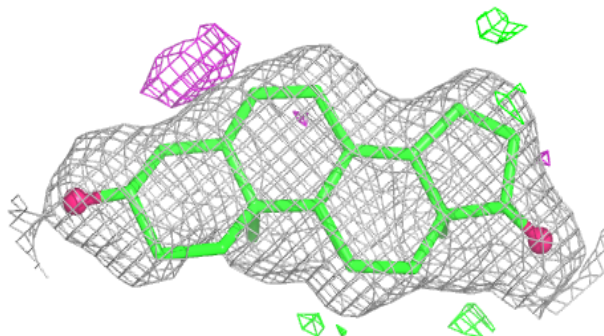
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	B81	E	601	21/21	0.86	0.13	29,40,49,54	0
3	B81	A	601	21/21	0.87	0.13	39,51,55,59	0
3	B81	F	601	21/21	0.88	0.11	22,33,39,42	0
3	B81	B	601	21/21	0.91	0.09	14,25,28,32	0

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.

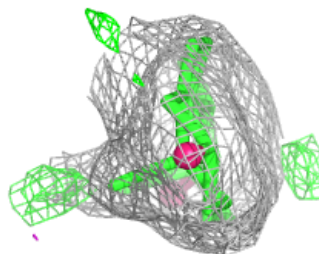
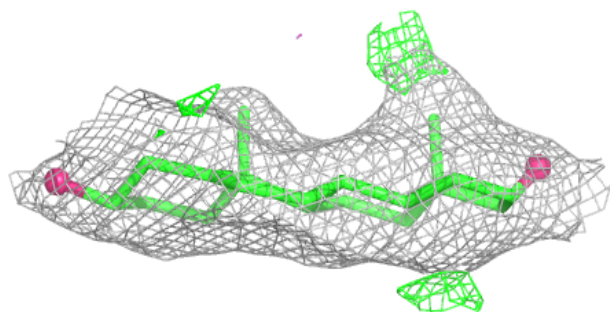
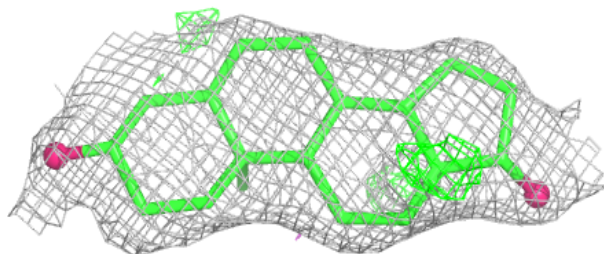


**Electron density around B81 E 601:**

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

**Electron density around B81 A 601:**

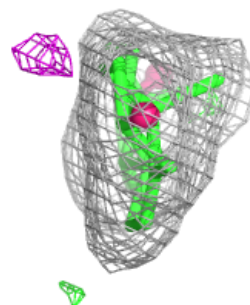
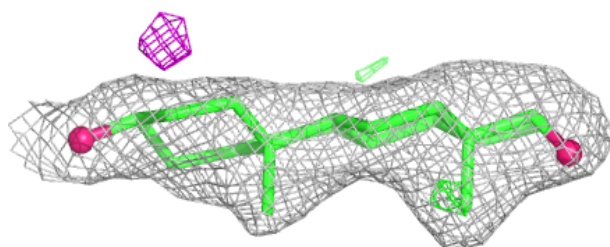
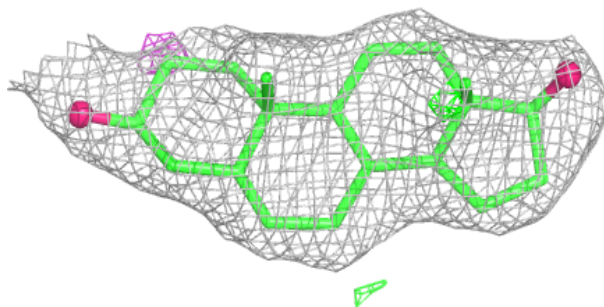
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



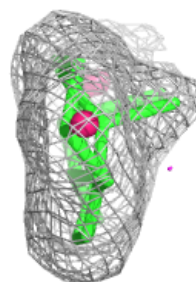
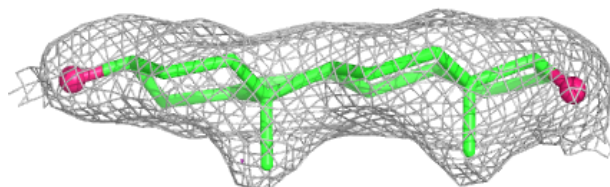
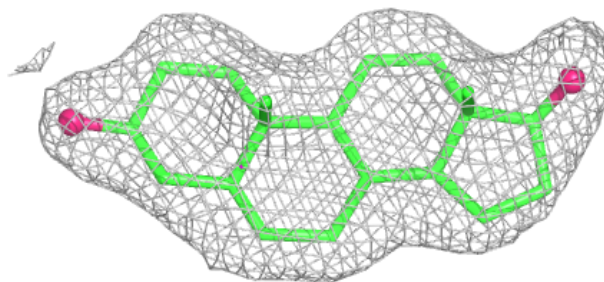


**Electron density around B81 F 601:**

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

**Electron density around B81 B 601:**

$2mF_o-DF_c$  (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.