



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2025 – 12:12 PM EDT

PDB ID : 9NEM / pdb_00009nem
Title : Structure of Unc119-Farnesylated peptide complex
Authors : Srivastava, D.; Sebag, J.A.; Artemyev, N.O.
Deposited on : 2025-02-20
Resolution : 2.49 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:

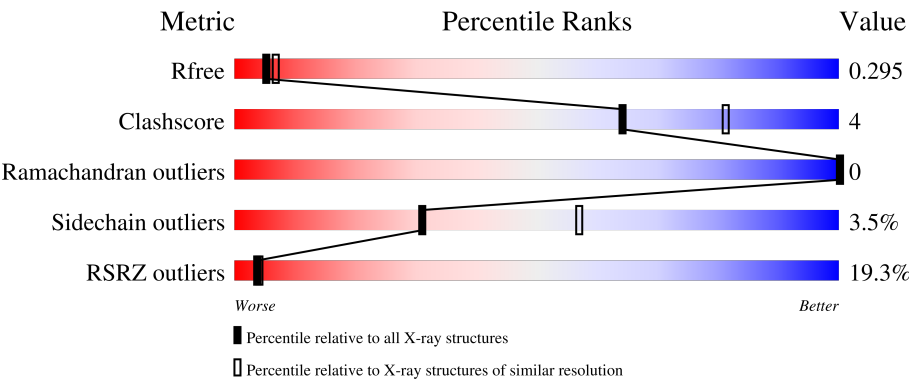
MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

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 2.49 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	196	<div><div>9%</div><div>74%</div><div>10%</div><div>•</div><div>15%</div></div>
1	B	196	<div><div>16%</div><div>78%</div><div>12%</div><div>•</div><div>9%</div></div>
1	C	196	<div><div>14%</div><div>74%</div><div>11%</div><div>•</div><div>15%</div></div>
1	D	196	<div><div>17%</div><div>78%</div><div>5%</div><div>•</div><div>15%</div></div>
1	E	196	<div><div>20%</div><div>73%</div><div>7%</div><div>•</div><div>19%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	196	<div><div></div><div>23%</div><div></div><div>71%</div><div></div><div>11%</div><div></div><div>18%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8490 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 Protein unc-119 homolog A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	3	0	0
			1385	892	233	253	7			
1	B	178	Total	C	N	O	S	10	0	0
			1482	951	253	271	7			
1	C	167	Total	C	N	O	S	5	0	0
			1385	892	233	253	7			
1	D	166	Total	C	N	O	S	6	1	0
			1387	893	235	252	7			
1	E	159	Total	C	N	O	S	0	0	0
			1334	861	223	243	7			
1	F	161	Total	C	N	O	S	4	0	0
			1344	866	224	247	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	initiating methionine	UNP Q13432
A	45	GLY	-	expression tag	UNP Q13432
A	46	SER	-	expression tag	UNP Q13432
A	47	SER	-	expression tag	UNP Q13432
A	48	HIS	-	expression tag	UNP Q13432
A	49	HIS	-	expression tag	UNP Q13432
A	50	HIS	-	expression tag	UNP Q13432
A	51	HIS	-	expression tag	UNP Q13432
A	52	HIS	-	expression tag	UNP Q13432
A	53	HIS	-	expression tag	UNP Q13432
A	54	SER	-	expression tag	UNP Q13432
A	55	SER	-	expression tag	UNP Q13432
B	44	MET	-	initiating methionine	UNP Q13432
B	45	GLY	-	expression tag	UNP Q13432
B	46	SER	-	expression tag	UNP Q13432
B	47	SER	-	expression tag	UNP Q13432
B	48	HIS	-	expression tag	UNP Q13432

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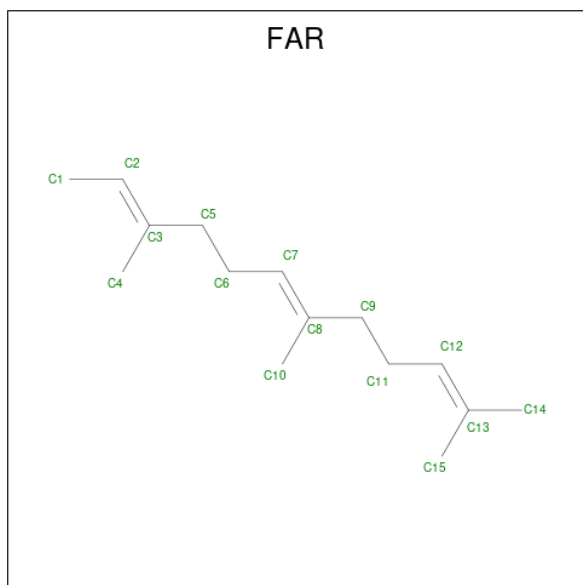
Chain	Residue	Modelled	Actual	Comment	Reference
B	49	HIS	-	expression tag	UNP Q13432
B	50	HIS	-	expression tag	UNP Q13432
B	51	HIS	-	expression tag	UNP Q13432
B	52	HIS	-	expression tag	UNP Q13432
B	53	HIS	-	expression tag	UNP Q13432
B	54	SER	-	expression tag	UNP Q13432
B	55	SER	-	expression tag	UNP Q13432
C	44	MET	-	initiating methionine	UNP Q13432
C	45	GLY	-	expression tag	UNP Q13432
C	46	SER	-	expression tag	UNP Q13432
C	47	SER	-	expression tag	UNP Q13432
C	48	HIS	-	expression tag	UNP Q13432
C	49	HIS	-	expression tag	UNP Q13432
C	50	HIS	-	expression tag	UNP Q13432
C	51	HIS	-	expression tag	UNP Q13432
C	52	HIS	-	expression tag	UNP Q13432
C	53	HIS	-	expression tag	UNP Q13432
C	54	SER	-	expression tag	UNP Q13432
C	55	SER	-	expression tag	UNP Q13432
D	44	MET	-	initiating methionine	UNP Q13432
D	45	GLY	-	expression tag	UNP Q13432
D	46	SER	-	expression tag	UNP Q13432
D	47	SER	-	expression tag	UNP Q13432
D	48	HIS	-	expression tag	UNP Q13432
D	49	HIS	-	expression tag	UNP Q13432
D	50	HIS	-	expression tag	UNP Q13432
D	51	HIS	-	expression tag	UNP Q13432
D	52	HIS	-	expression tag	UNP Q13432
D	53	HIS	-	expression tag	UNP Q13432
D	54	SER	-	expression tag	UNP Q13432
D	55	SER	-	expression tag	UNP Q13432
E	44	MET	-	initiating methionine	UNP Q13432
E	45	GLY	-	expression tag	UNP Q13432
E	46	SER	-	expression tag	UNP Q13432
E	47	SER	-	expression tag	UNP Q13432
E	48	HIS	-	expression tag	UNP Q13432
E	49	HIS	-	expression tag	UNP Q13432
E	50	HIS	-	expression tag	UNP Q13432
E	51	HIS	-	expression tag	UNP Q13432
E	52	HIS	-	expression tag	UNP Q13432
E	53	HIS	-	expression tag	UNP Q13432
E	54	SER	-	expression tag	UNP Q13432

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Chain	Residue	Modelled	Actual	Comment	Reference
E	55	SER	-	expression tag	UNP Q13432
F	44	MET	-	initiating methionine	UNP Q13432
F	45	GLY	-	expression tag	UNP Q13432
F	46	SER	-	expression tag	UNP Q13432
F	47	SER	-	expression tag	UNP Q13432
F	48	HIS	-	expression tag	UNP Q13432
F	49	HIS	-	expression tag	UNP Q13432
F	50	HIS	-	expression tag	UNP Q13432
F	51	HIS	-	expression tag	UNP Q13432
F	52	HIS	-	expression tag	UNP Q13432
F	53	HIS	-	expression tag	UNP Q13432
F	54	SER	-	expression tag	UNP Q13432
F	55	SER	-	expression tag	UNP Q13432

- Molecule 2 is FARNESYL (CCD ID: FAR) (formula: $C_{15}H_{26}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 15 15	0	0
2	B	1	Total C 15 15	0	0
2	C	1	Total C 15 15	0	0
2	D	1	Total C 15 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C 15 15	0	0

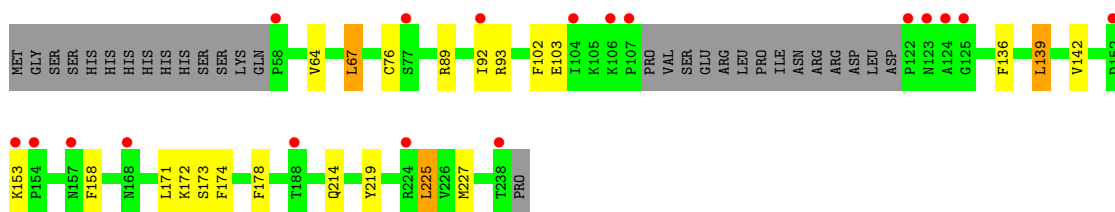
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	35	Total O 35 35	0	0
3	B	23	Total O 23 23	0	0
3	C	18	Total O 18 18	0	0
3	D	9	Total O 9 9	0	0
3	E	4	Total O 4 4	0	0
3	F	9	Total O 9 9	0	0

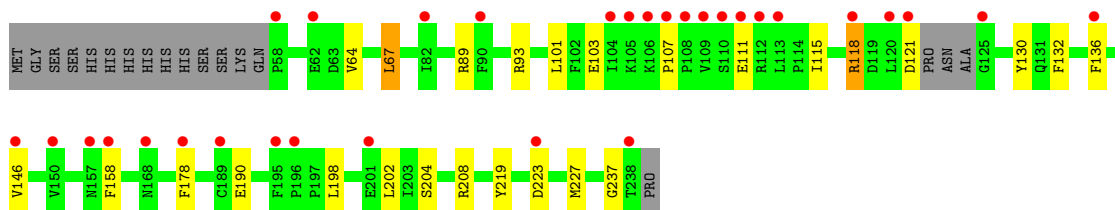
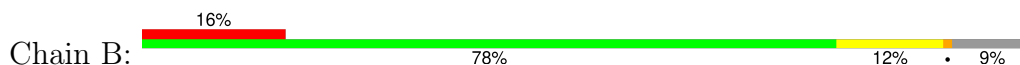
3 Residue-property plots [i](#)

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.

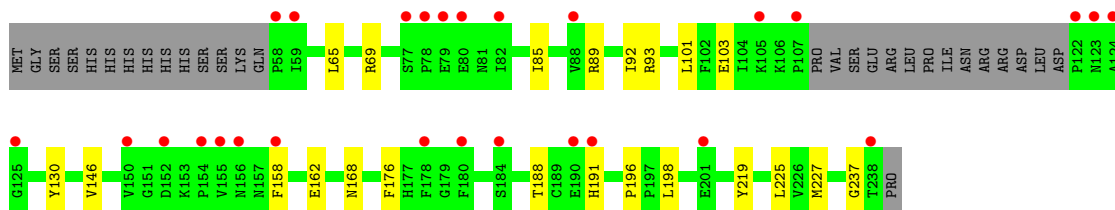
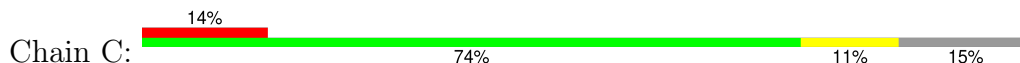
• Molecule 1: Protein unc-119 homolog A



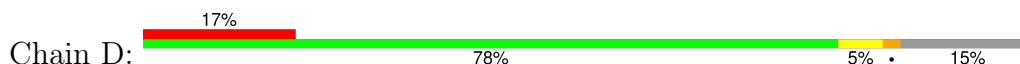
• Molecule 1: Protein unc-119 homolog A

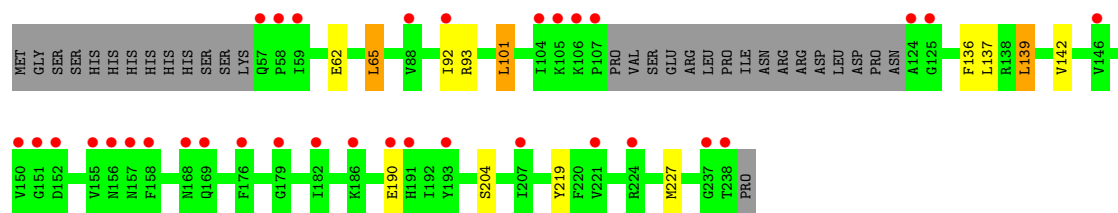


• Molecule 1: Protein unc-119 homolog A

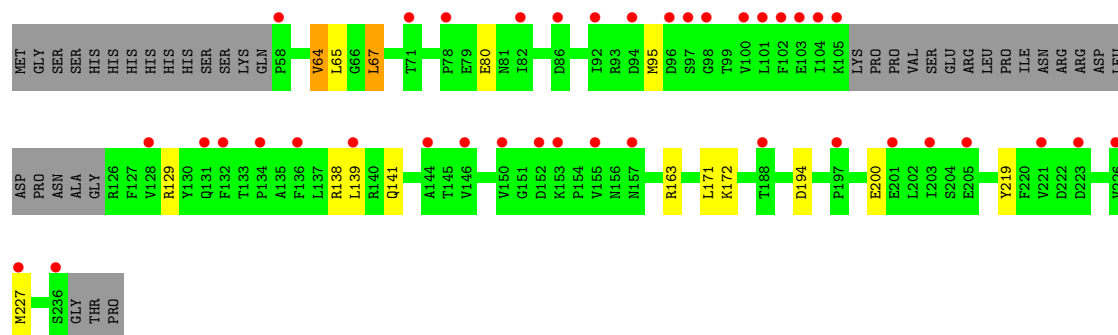
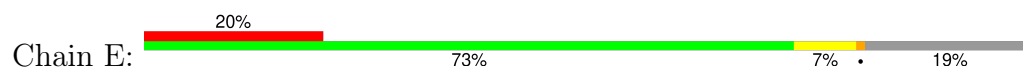


• Molecule 1: Protein unc-119 homolog A

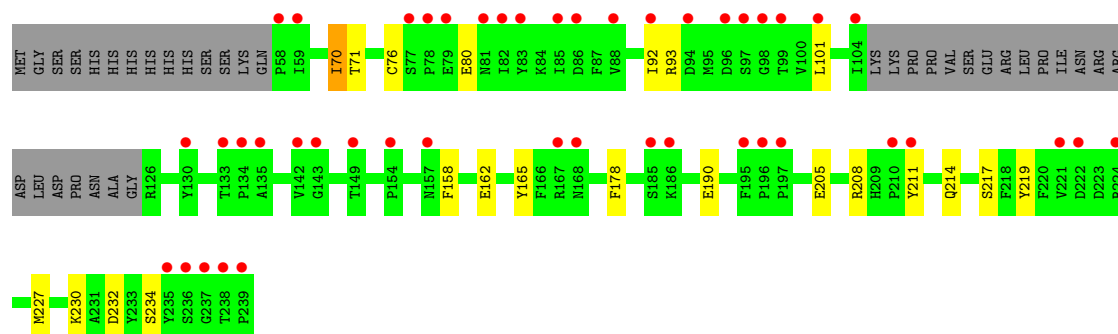




● Molecule 1: Protein unc-119 homolog A



● Molecule 1: Protein unc-119 homolog A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.16Å 81.04Å 192.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 2.49 49.82 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.82-2.49) 98.3 (49.82-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.263 , 0.295 0.264 , 0.295	Depositor DCC
R_{free} test set	2184 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8490	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.36% 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: FAR

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	0.14	0/1424	0.32	0/1921
1	B	0.14	0/1522	0.31	0/2054
1	C	0.13	0/1424	0.31	0/1921
1	D	0.13	0/1428	0.30	0/1926
1	E	0.12	0/1371	0.28	0/1849
1	F	0.12	0/1382	0.29	0/1865
All	All	0.13	0/8551	0.30	0/11536

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	1385	0	1334	12	0
1	B	1482	0	1435	15	0
1	C	1385	0	1334	12	0
1	D	1387	0	1340	6	0
1	E	1334	0	1282	7	0
1	F	1344	0	1286	11	0
2	A	15	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	26	2	0
2	C	15	0	26	3	0
2	D	15	0	26	0	0
2	E	15	0	26	0	0
3	A	35	0	0	1	0
3	B	23	0	0	1	0
3	C	18	0	0	1	0
3	D	9	0	0	1	0
3	E	4	0	0	0	0
3	F	9	0	0	0	0
All	All	8490	0	8141	62	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 4.

All (62) 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:F:76:CYS:HB2	1:F:80:GLU:HG3	1.79	0.64
1:A:76:CYS:HB3	1:A:225:LEU:HD13	1.80	0.63
1:C:89:ARG:NH1	1:C:103:GLU:OE2	2.32	0.62
1:F:158:PHE:HB3	1:F:178:PHE:HB2	1.82	0.61
1:F:219:TYR:HB2	1:F:227:MET:HB2	1.83	0.61
1:F:70:ILE:HG13	1:F:214:GLN:HB2	1.83	0.60
1:D:136:PHE:HA	1:D:139:LEU:HD22	1.85	0.59
1:E:67:LEU:O	1:E:163:ARG:NH2	2.32	0.58
1:A:136:PHE:HA	1:A:139:LEU:HD22	1.87	0.56
1:A:89:ARG:NH1	1:A:103:GLU:OE2	2.39	0.55
1:A:219:TYR:HB2	1:A:227:MET:HB2	1.89	0.55
1:B:107:PRO:HG2	1:B:111:GLU:HG3	1.88	0.54
1:C:162:GLU:OE2	2:C:301:FAR:H42	2.08	0.53
1:B:101:LEU:HB3	1:B:136:PHE:CZ	2.43	0.52
1:A:64:VAL:HA	1:A:67:LEU:HD22	1.92	0.51
1:B:89:ARG:NH1	1:B:103:GLU:OE2	2.44	0.50
1:A:92:ILE:HD12	1:A:102:PHE:HB3	1.93	0.50
1:C:93:ARG:NH1	3:C:401:HOH:O	2.35	0.49
1:C:196:PRO:HD2	2:C:301:FAR:H141	1.93	0.49
1:C:219:TYR:HB2	1:C:227:MET:HB2	1.95	0.49
1:F:205:GLU:OE2	1:F:208:ARG:NH1	2.44	0.49
1:F:71:THR:OG1	1:F:230:LYS:NZ	2.45	0.49
1:C:69:ARG:HG2	1:C:168:ASN:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:VAL:HA	1:E:67:LEU:HD22	1.95	0.48
1:F:93:ARG:NH1	1:F:190:GLU:OE2	2.44	0.48
1:B:219:TYR:HB2	1:B:227:MET:HB2	1.95	0.48
1:C:130:TYR:CE2	2:C:301:FAR:H2	2.49	0.47
1:D:219:TYR:HB2	1:D:227:MET:HB2	1.96	0.47
1:E:95:MET:HG3	1:E:141:GLN:HG2	1.96	0.47
1:C:85:ILE:HD13	1:C:158:PHE:CZ	2.50	0.47
1:B:237:GLY:HA3	1:C:237:GLY:HA3	1.97	0.47
1:B:132:PHE:HB3	1:B:136:PHE:CD1	2.50	0.46
1:E:219:TYR:HB2	1:E:227:MET:HB2	1.98	0.46
1:F:211:TYR:CE1	1:F:234:SER:HB2	2.51	0.46
1:E:138:ARG:NH1	1:E:200:GLU:OE2	2.48	0.46
1:F:92:ILE:HG22	1:F:101:LEU:HD12	1.98	0.46
1:A:153:LYS:H	1:A:153:LYS:HE2	1.82	0.45
1:D:139:LEU:HD12	1:D:139:LEU:HA	1.85	0.45
1:D:93[B]:ARG:NH2	3:D:401:HOH:O	2.45	0.45
1:B:64:VAL:HA	1:B:67:LEU:HD22	1.98	0.45
1:F:162:GLU:OE1	1:F:217:SER:OG	2.35	0.45
1:B:130:TYR:CE2	2:B:301:FAR:H2	2.53	0.44
1:C:92:ILE:HG22	1:C:101:LEU:HD12	1.99	0.44
1:B:158:PHE:HB3	1:B:178:PHE:HB2	2.00	0.44
1:B:204:SER:O	1:B:208:ARG:HG3	2.18	0.43
1:B:118:ARG:HA	1:B:118:ARG:HD2	1.76	0.43
1:D:65:LEU:HD12	1:D:65:LEU:HA	1.83	0.43
1:A:172:LYS:HG3	1:A:173:SER:N	2.34	0.43
1:A:214:GLN:NE2	3:A:406:HOH:O	2.51	0.43
2:A:301:FAR:H61	2:A:301:FAR:H2	1.75	0.43
1:C:176:PHE:HB3	1:C:191:HIS:CE1	2.54	0.42
1:B:101:LEU:HB3	1:B:136:PHE:HZ	1.85	0.42
1:A:93:ARG:NH2	1:B:115:ILE:HG21	2.35	0.42
1:B:121:ASP:N	1:B:121:ASP:OD1	2.53	0.42
2:B:301:FAR:H41	2:B:301:FAR:H61	1.75	0.42
1:A:158:PHE:HB3	1:A:178:PHE:HB2	2.01	0.42
1:C:188:THR:O	1:E:129:ARG:NH1	2.52	0.42
1:B:93:ARG:HD2	3:B:401:HOH:O	2.19	0.41
1:D:92:ILE:HG22	1:D:101:LEU:HB2	2.02	0.41
1:A:172:LYS:HG2	1:A:174:PHE:CZ	2.57	0.40
1:E:172:LYS:NZ	1:E:194:ASP:O	2.28	0.40
1:F:70:ILE:HG12	1:F:165:TYR:CD1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	163/196 (83%)	161 (99%)	2 (1%)	0	100	100
1	B	174/196 (89%)	172 (99%)	2 (1%)	0	100	100
1	C	163/196 (83%)	158 (97%)	5 (3%)	0	100	100
1	D	163/196 (83%)	161 (99%)	2 (1%)	0	100	100
1	E	155/196 (79%)	153 (99%)	2 (1%)	0	100	100
1	F	157/196 (80%)	155 (99%)	2 (1%)	0	100	100
All	All	975/1176 (83%)	960 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	154/182 (85%)	149 (97%)	5 (3%)	34	60
1	B	166/182 (91%)	159 (96%)	7 (4%)	25	49
1	C	154/182 (85%)	150 (97%)	4 (3%)	41	68
1	D	154/182 (85%)	146 (95%)	8 (5%)	19	39
1	E	149/182 (82%)	143 (96%)	6 (4%)	27	51
1	F	150/182 (82%)	148 (99%)	2 (1%)	65	85
All	All	927/1092 (85%)	895 (96%)	32 (4%)	31	57

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	139	LEU
1	A	142	VAL
1	A	171	LEU
1	A	225	LEU
1	B	67	LEU
1	B	118	ARG
1	B	146	VAL
1	B	190	GLU
1	B	198	LEU
1	B	202	LEU
1	B	223	ASP
1	C	65	LEU
1	C	146	VAL
1	C	198	LEU
1	C	225	LEU
1	D	62	GLU
1	D	65	LEU
1	D	101	LEU
1	D	137	LEU
1	D	139	LEU
1	D	142	VAL
1	D	190	GLU
1	D	204	SER
1	E	64	VAL
1	E	65	LEU
1	E	67	LEU
1	E	80	GLU
1	E	139	LEU
1	E	171	LEU
1	F	70	ILE
1	F	232	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	209	HIS
1	B	156	ASN
1	B	214	GLN
1	C	123	ASN

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Mol	Chain	Res	Type
1	C	131	GLN
1	C	229	ASN
1	E	177	HIS
1	F	177	HIS
1	F	191	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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAR	B	301	-	14,14,14	0.22	0	15,16,16	0.49	0
2	FAR	A	301	-	14,14,14	0.30	0	15,16,16	0.48	0
2	FAR	C	301	-	14,14,14	0.20	0	15,16,16	0.72	0
2	FAR	E	301	-	14,14,14	0.27	0	15,16,16	0.56	0
2	FAR	D	301	-	14,14,14	0.32	0	15,16,16	0.84	0

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	FAR	B	301	-	-	4/14/14/14	-
2	FAR	A	301	-	-	1/14/14/14	-
2	FAR	C	301	-	-	3/14/14/14	-
2	FAR	E	301	-	-	3/14/14/14	-
2	FAR	D	301	-	-	4/14/14/14	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	FAR	C3-C5-C6-C7
2	D	301	FAR	C10-C8-C9-C11
2	B	301	FAR	C4-C3-C5-C6
2	E	301	FAR	C4-C3-C5-C6
2	B	301	FAR	C2-C3-C5-C6
2	D	301	FAR	C7-C8-C9-C11
2	E	301	FAR	C2-C3-C5-C6
2	C	301	FAR	C3-C5-C6-C7
2	E	301	FAR	C3-C5-C6-C7
2	B	301	FAR	C3-C5-C6-C7
2	B	301	FAR	C12-C11-C9-C8
2	D	301	FAR	C12-C11-C9-C8
2	C	301	FAR	C10-C8-C9-C11
2	C	301	FAR	C7-C8-C9-C11
2	D	301	FAR	C3-C5-C6-C7

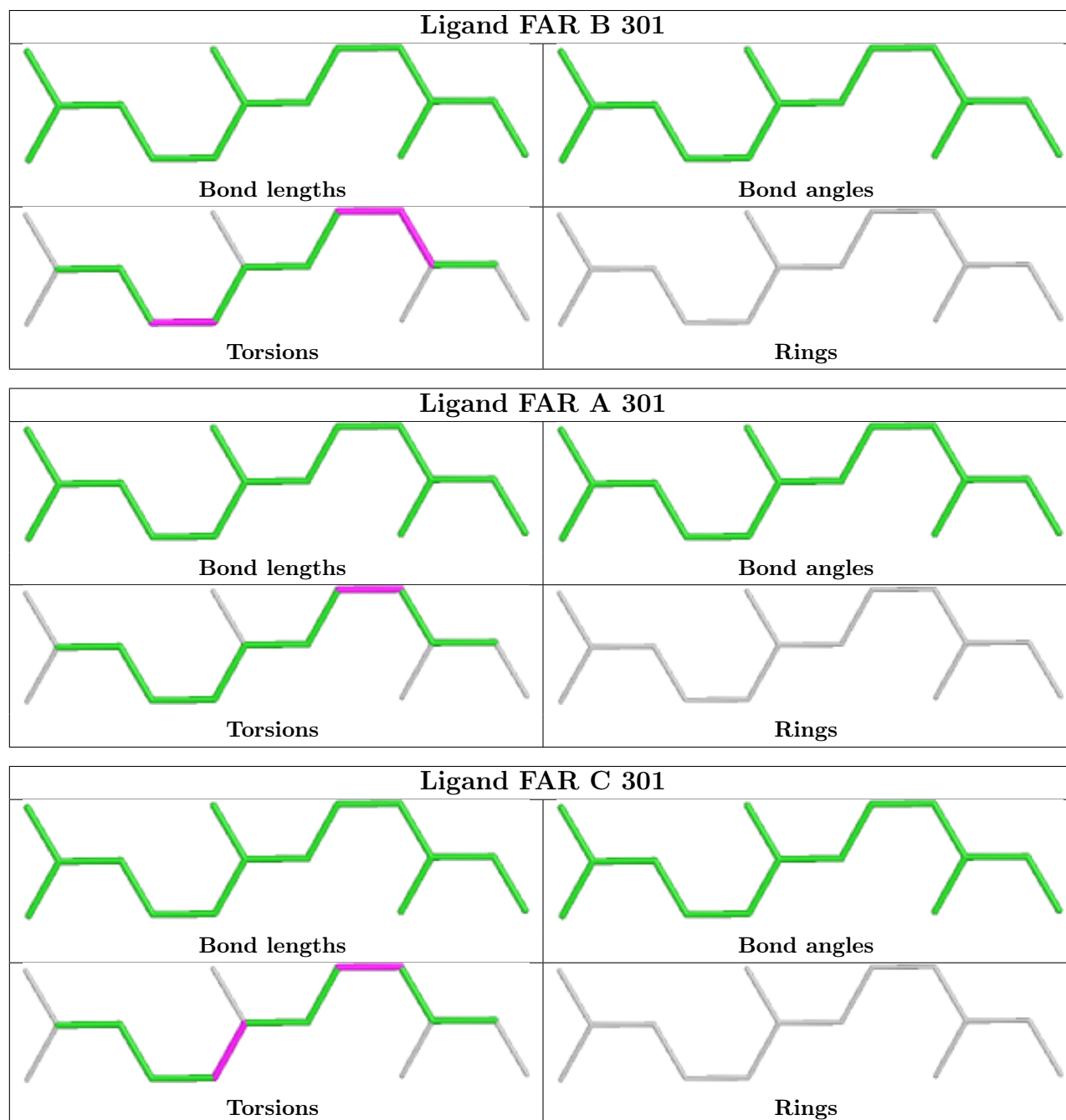
There are no ring outliers.

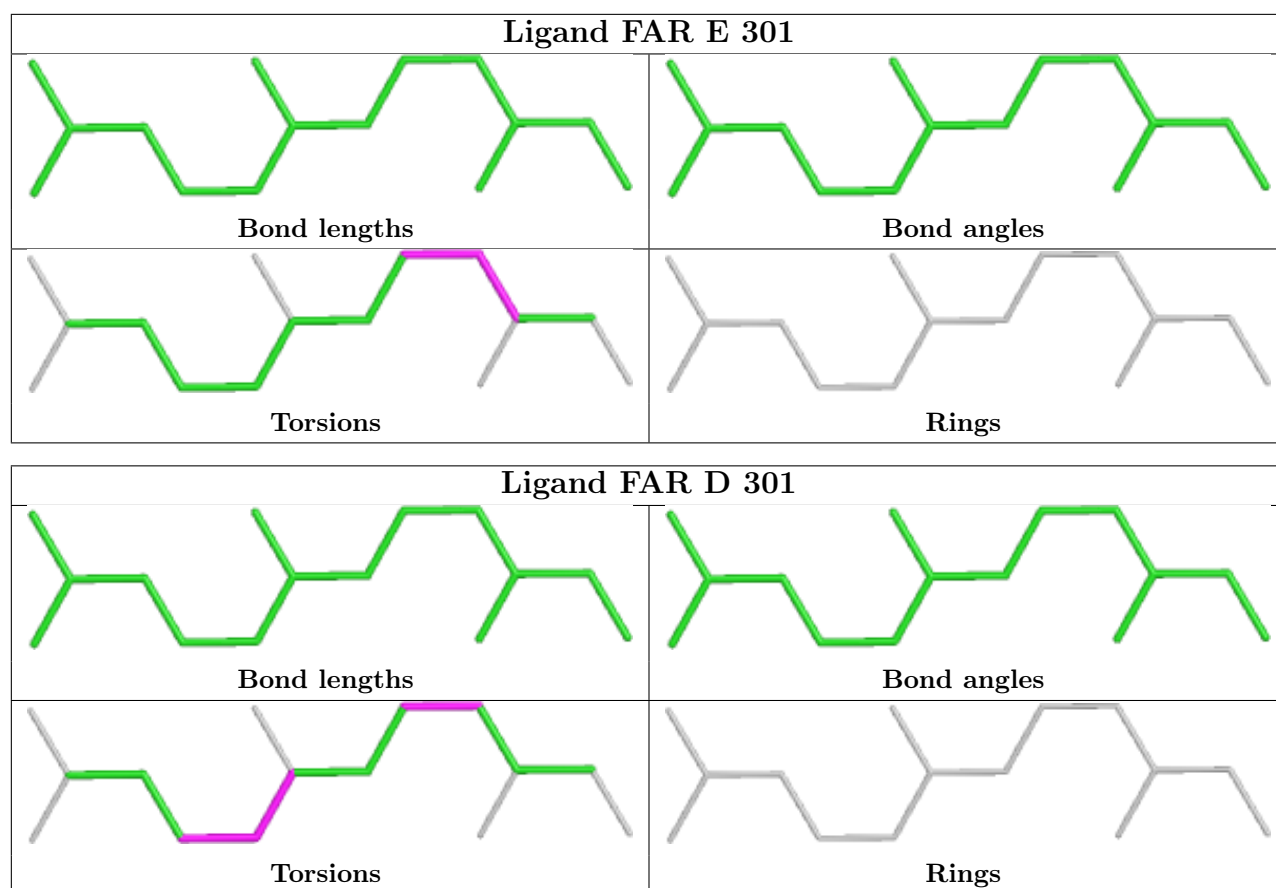
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	FAR	2	0
2	A	301	FAR	1	0
2	C	301	FAR	3	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	167/196 (85%)	1.04	18 (10%)	12 11	29, 38, 59, 83	1 (0%)
1	B	178/196 (90%)	1.14	31 (17%)	5 5	14, 39, 66, 97	2 (1%)
1	C	167/196 (85%)	1.19	27 (16%)	5 5	26, 42, 66, 90	1 (0%)
1	D	166/196 (84%)	1.31	33 (19%)	3 4	22, 45, 69, 94	2 (1%)
1	E	159/196 (81%)	1.50	39 (24%)	2 2	35, 52, 75, 92	0
1	F	161/196 (82%)	1.54	45 (27%)	2 2	30, 54, 70, 103	1 (0%)
All	All	998/1176 (84%)	1.28	193 (19%)	4 4	14, 44, 71, 103	7 (0%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	THR	5.9
1	A	107	PRO	5.9
1	B	108	PRO	5.3
1	A	124	ALA	5.1
1	C	107	PRO	4.9
1	D	238	THR	4.8
1	B	112	ARG	4.7
1	B	118	ARG	4.6
1	F	238	THR	4.6
1	D	57	GLN	4.5
1	A	122	PRO	4.5
1	A	238	THR	4.4
1	C	122	PRO	4.4
1	E	155	VAL	4.4
1	D	107	PRO	4.3
1	D	125	GLY	4.1
1	B	58	PRO	4.1
1	B	120	LEU	4.0
1	F	104	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	238	THR	3.9
1	A	58	PRO	3.8
1	F	239	PRO	3.8
1	E	101	LEU	3.7
1	C	79	GLU	3.7
1	B	121	ASP	3.7
1	D	58	PRO	3.5
1	B	111	GLU	3.5
1	D	152	ASP	3.4
1	F	237	GLY	3.4
1	C	190	GLU	3.4
1	B	136	PHE	3.4
1	A	123	ASN	3.4
1	B	109	VAL	3.4
1	C	180	PHE	3.3
1	E	92	ILE	3.3
1	D	176	PHE	3.3
1	E	104	ILE	3.2
1	F	97	SER	3.2
1	A	125	GLY	3.2
1	E	150	VAL	3.2
1	E	58	PRO	3.2
1	B	125	GLY	3.2
1	C	124	ALA	3.1
1	F	236	SER	3.1
1	C	58	PRO	3.1
1	B	62	GLU	3.1
1	E	153	LYS	3.1
1	B	104	ILE	3.1
1	E	188	THR	3.1
1	F	149	THR	3.1
1	F	92	ILE	3.0
1	E	97	SER	3.0
1	E	82	ILE	3.0
1	D	124	ALA	3.0
1	C	77	SER	3.0
1	D	151	GLY	3.0
1	E	98	GLY	2.9
1	D	182	ILE	2.9
1	D	191	HIS	2.9
1	E	105	LYS	2.9
1	D	104	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	236	SER	2.9
1	D	105	LYS	2.9
1	D	106	LYS	2.9
1	F	195	PHE	2.8
1	F	196	PRO	2.8
1	E	103	GLU	2.8
1	A	157	ASN	2.8
1	C	59	ILE	2.8
1	D	92	ILE	2.8
1	C	154	PRO	2.8
1	B	110	SER	2.8
1	A	168	ASN	2.8
1	F	134	PRO	2.8
1	E	102	PHE	2.8
1	C	201	GLU	2.7
1	B	90	PHE	2.7
1	D	155	VAL	2.7
1	B	105	LYS	2.7
1	C	88	VAL	2.7
1	C	155	VAL	2.7
1	F	99	THR	2.7
1	F	81	ASN	2.7
1	F	79	GLU	2.7
1	C	152	ASP	2.7
1	D	168	ASN	2.7
1	F	98	GLY	2.7
1	A	224	ARG	2.6
1	B	106	LYS	2.6
1	F	197	PRO	2.6
1	B	107	PRO	2.6
1	F	133	THR	2.6
1	C	123	ASN	2.6
1	E	205	GLU	2.6
1	F	130	TYR	2.6
1	D	150	VAL	2.5
1	F	78	PRO	2.5
1	F	88	VAL	2.5
1	E	197	PRO	2.5
1	A	104	ILE	2.5
1	C	82	ILE	2.5
1	D	190	GLU	2.5
1	F	235	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	100	VAL	2.5
1	C	78	PRO	2.5
1	F	58	PRO	2.5
1	F	210	PRO	2.5
1	C	191	HIS	2.5
1	D	146	VAL	2.5
1	D	221	VAL	2.5
1	A	92	ILE	2.5
1	A	188	THR	2.5
1	E	152	ASP	2.5
1	D	169	GLN	2.4
1	D	186	LYS	2.4
1	E	227	MET	2.4
1	F	186	LYS	2.4
1	F	96	ASP	2.4
1	F	168	ASN	2.4
1	B	150	VAL	2.4
1	E	144	ALA	2.4
1	E	201	GLU	2.4
1	C	156	ASN	2.4
1	D	88	VAL	2.4
1	E	78	PRO	2.4
1	D	179	GLY	2.4
1	E	223	ASP	2.3
1	B	201	GLU	2.3
1	C	150	VAL	2.3
1	E	139	LEU	2.3
1	B	158	PHE	2.3
1	E	86	ASP	2.3
1	E	96	ASP	2.3
1	F	94	ASP	2.3
1	A	77	SER	2.3
1	B	195	PHE	2.3
1	D	157	ASN	2.3
1	D	193	TYR	2.3
1	B	146	VAL	2.3
1	F	135	ALA	2.3
1	B	223	ASP	2.3
1	F	222	ASP	2.3
1	F	157	ASN	2.3
1	E	134	PRO	2.3
1	C	80	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	237	GLY	2.2
1	C	184	SER	2.2
1	D	224	ARG	2.2
1	B	157	ASN	2.2
1	A	153	LYS	2.2
1	C	105	LYS	2.2
1	E	132	PHE	2.2
1	B	168	ASN	2.2
1	E	203	ILE	2.2
1	F	211	TYR	2.2
1	F	101	LEU	2.2
1	B	189	CYS	2.2
1	E	136	PHE	2.2
1	F	86	ASP	2.2
1	E	221	VAL	2.2
1	A	106	LYS	2.2
1	B	113	LEU	2.2
1	B	196	PRO	2.2
1	F	154	PRO	2.2
1	E	131	GLN	2.2
1	B	82	ILE	2.2
1	D	59	ILE	2.2
1	B	178	PHE	2.1
1	E	157	ASN	2.1
1	F	221	VAL	2.1
1	C	125	GLY	2.1
1	E	71	THR	2.1
1	A	154	PRO	2.1
1	E	94	ASP	2.1
1	E	128	VAL	2.1
1	F	142	VAL	2.1
1	F	143	GLY	2.1
1	F	77	SER	2.1
1	A	152	ASP	2.1
1	F	82	ILE	2.1
1	F	85	ILE	2.1
1	E	146	VAL	2.1
1	F	185	SER	2.1
1	D	156	ASN	2.1
1	E	226	VAL	2.0
1	F	224	ARG	2.0
1	F	83	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	207	ILE	2.0
1	C	158	PHE	2.0
1	C	178	PHE	2.0
1	D	158	PHE	2.0
1	F	59	ILE	2.0
1	F	167	ARG	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](#)

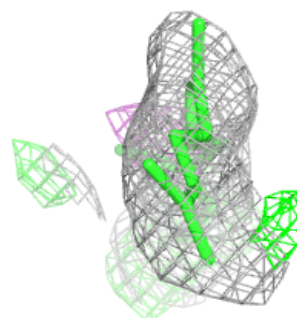
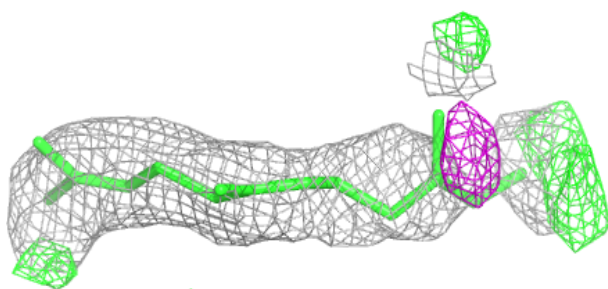
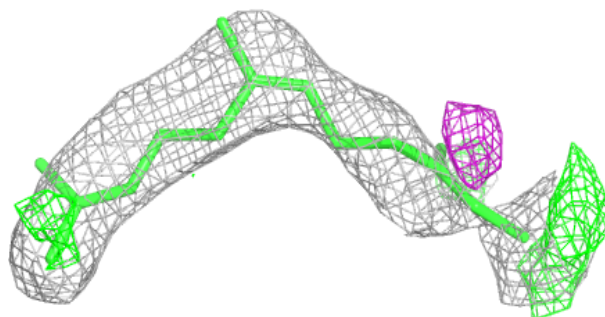
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAR	C	301	15/15	0.59	0.28	38,45,57,58	0
2	FAR	D	301	15/15	0.69	0.25	49,54,59,59	0
2	FAR	E	301	15/15	0.69	0.24	46,50,55,56	0
2	FAR	B	301	15/15	0.71	0.24	38,44,47,49	0
2	FAR	A	301	15/15	0.79	0.20	43,46,51,51	0

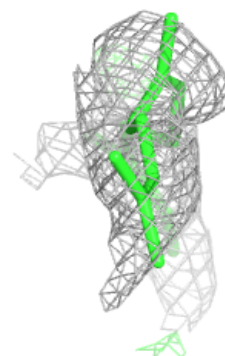
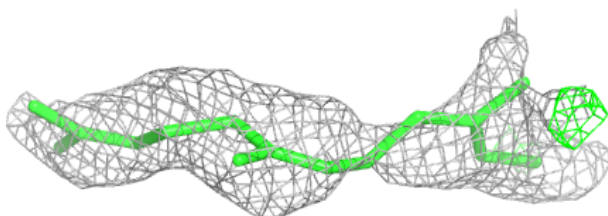
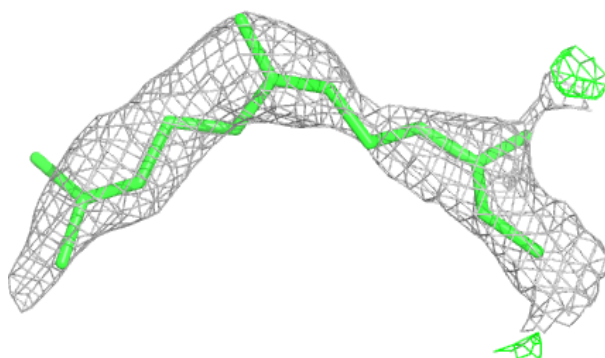
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAR C 301:

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

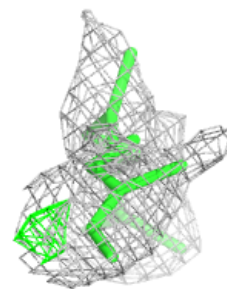
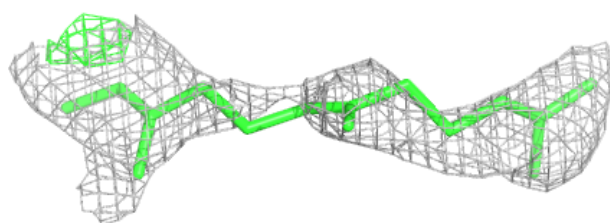
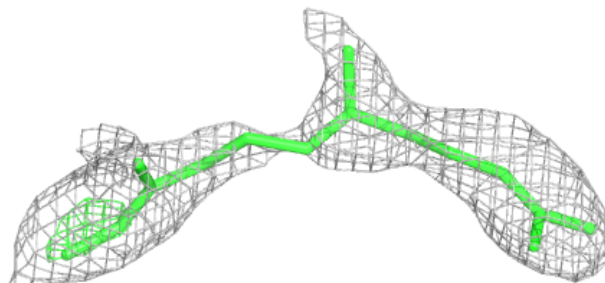
**Electron density around FAR D 301:**

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

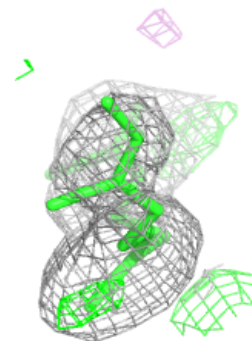
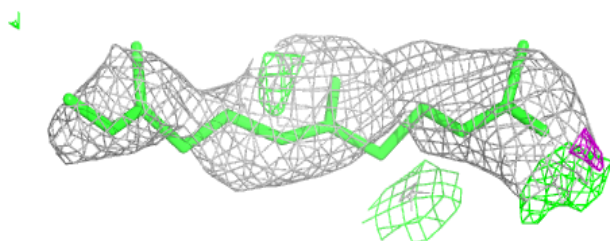
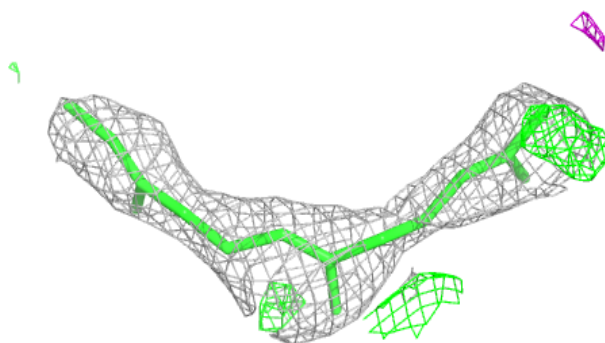


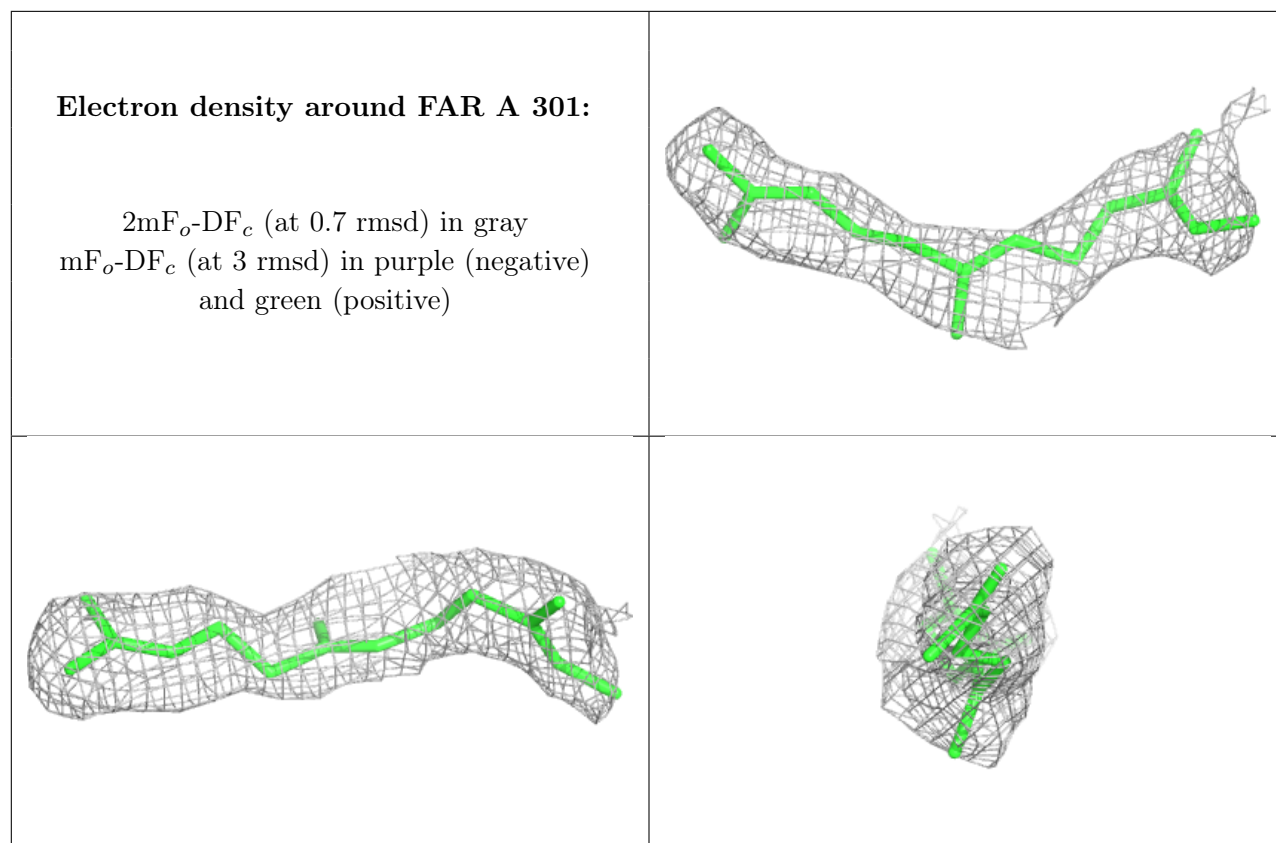
Electron density around FAR E 301:

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

**Electron density around FAR B 301:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.