



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:30 pm BST

PDB ID : 4PLE
Title : Human Nuclear Receptor Liver Receptor Homologue-1, LRH-1, Bound to an E. Coli Phospholipid and a Fragment of TIF-2
Authors : Ortlund, E.A.; Musille, P.M.
Deposited on : 2014-05-16
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

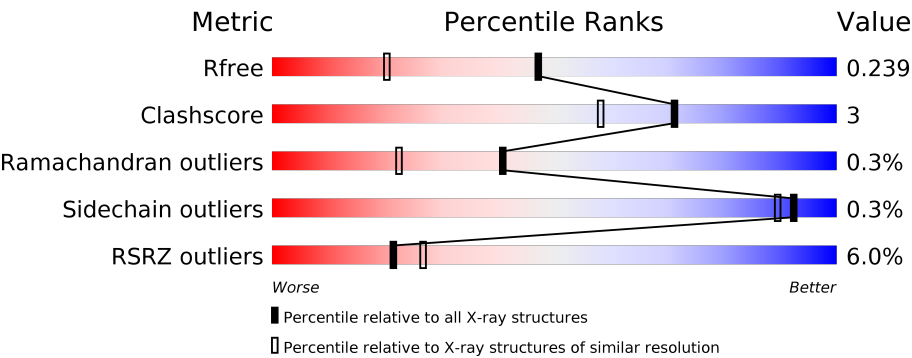
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



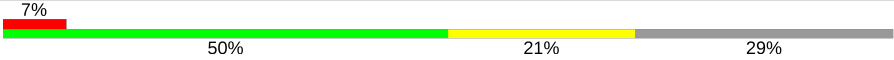

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	245	<div><div>9%</div><div>89%</div><div>9%</div><div></div></div>
1	C	245	<div><div>4%</div><div>89%</div><div>9%</div><div></div></div>
1	E	245	<div><div>6%</div><div>87%</div><div>10%</div><div></div></div>
1	G	245	<div><div>4%</div><div>91%</div><div>7%</div><div></div></div>
2	B	14	<div><div></div><div>57%</div><div>7%</div><div>36%</div></div>
2	D	14	<div><div>14%</div><div>64%</div><div>7%</div><div>29%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	14	
2	H	14	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9019 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 Nuclear receptor subfamily 5 group A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1953	1252	327	361	13			
1	C	239	Total	C	N	O	S	0	1	0
			1945	1249	324	358	14			
1	E	241	Total	C	N	O	S	0	1	0
			1958	1256	327	361	14			
1	G	241	Total	C	N	O	S	0	1	0
			1958	1256	327	361	14			

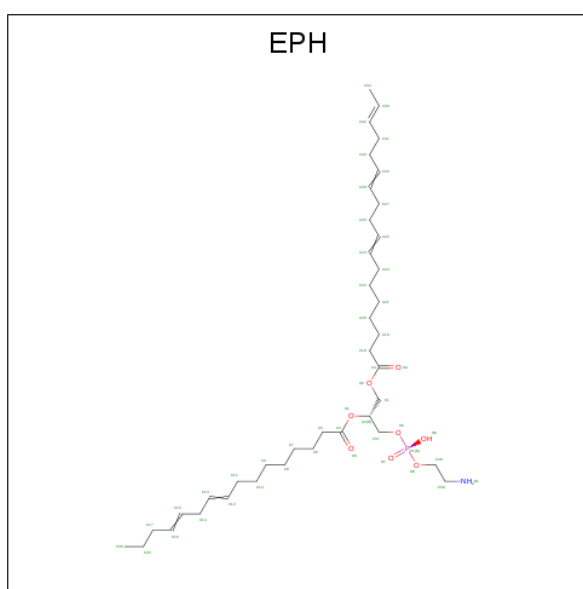
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	ALA	-	expression tag	UNP O00482
A	298	ALA	-	expression tag	UNP O00482
A	299	ALA	-	expression tag	UNP O00482
A	300	SER	-	expression tag	UNP O00482
C	297	ALA	-	expression tag	UNP O00482
C	298	ALA	-	expression tag	UNP O00482
C	299	ALA	-	expression tag	UNP O00482
C	300	SER	-	expression tag	UNP O00482
E	297	ALA	-	expression tag	UNP O00482
E	298	ALA	-	expression tag	UNP O00482
E	299	ALA	-	expression tag	UNP O00482
E	300	SER	-	expression tag	UNP O00482
G	297	ALA	-	expression tag	UNP O00482
G	298	ALA	-	expression tag	UNP O00482
G	299	ALA	-	expression tag	UNP O00482
G	300	SER	-	expression tag	UNP O00482

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

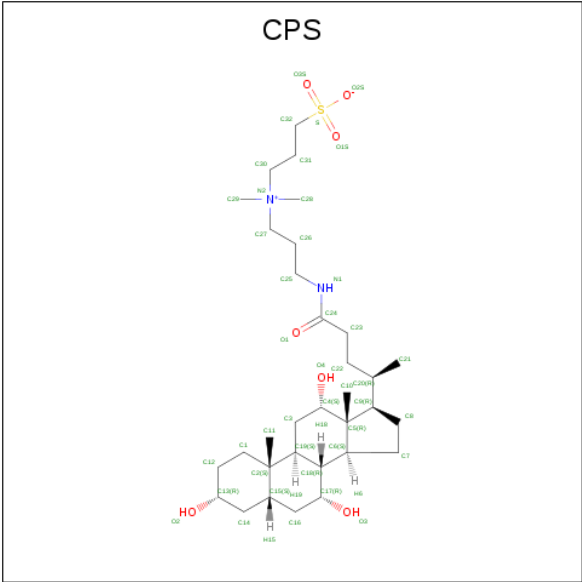
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			76	50	13	13			
2	D	10	Total	C	N	O	0	0	0
			85	56	15	14			
2	F	10	Total	C	N	O	0	0	0
			85	56	15	14			
2	H	10	Total	C	N	O	0	0	0
			85	56	15	14			

- Molecule 3 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			47	38	8	1		
3	C	1	Total	C	O	P	0	0
			47	38	8	1		
3	E	1	Total	C	O	P	0	0
			47	38	8	1		
3	G	1	Total	C	O	P	0	0
			47	38	8	1		

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O			
			24	21	3	0	0	
4	A	1	Total	C	O			
			22	19	3	0	0	
4	A	1	Total	C	N	O		
			29	24	1	4	0	
4	C	1	Total	C	O			
			25	22	3	0	0	
4	C	1	Total	C	O			
			24	21	3	0	0	
4	E	1	Total	C	O			
			26	23	3	0	0	
4	E	1	Total	C	N	O		
			31	26	1	4	0	
4	E	1	Total	C	O			
			24	21	3	0	0	
4	E	1	Total	C	O			
			23	20	3	0	0	
4	E	1	Total	C	O			
			24	21	3	0	0	
4	G	1	Total	C	N	O		
			30	25	1	4	0	
4	G	1	Total	C	O			
			23	20	3	0	0	

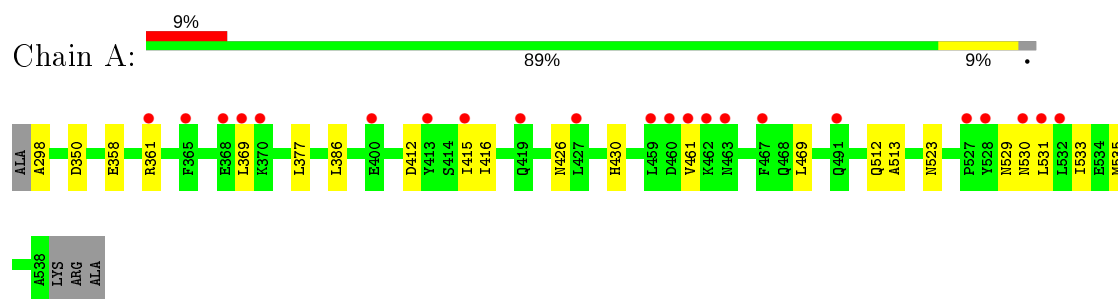
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total 90	O 90	0	0
5	C	103	Total 103	O 103	0	0
5	D	1	Total 1	O 1	0	0
5	E	94	Total 94	O 94	0	0
5	G	92	Total 92	O 92	0	0
5	H	1	Total 1	O 1	0	0

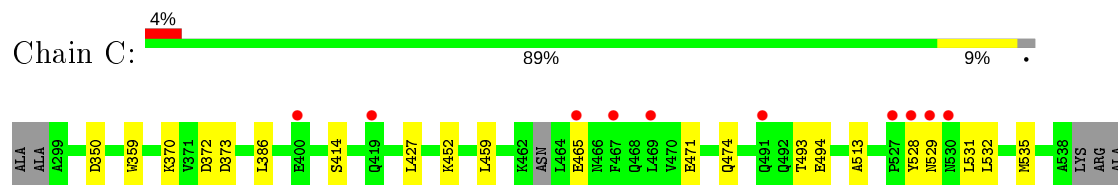
3 Residue-property plots [i](#)

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

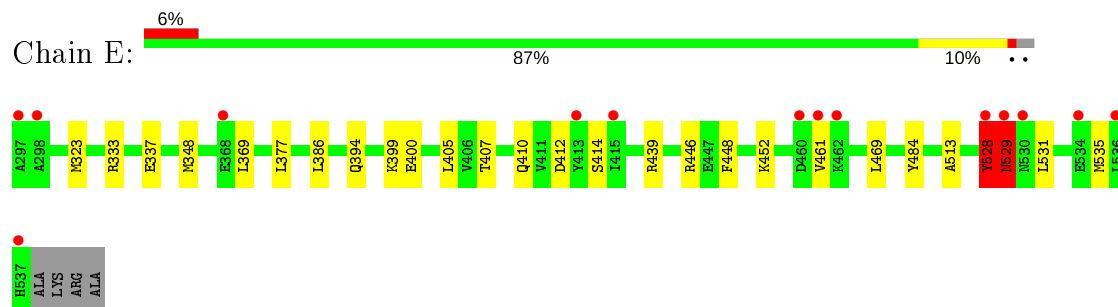
- Molecule 1: Nuclear receptor subfamily 5 group A member 2



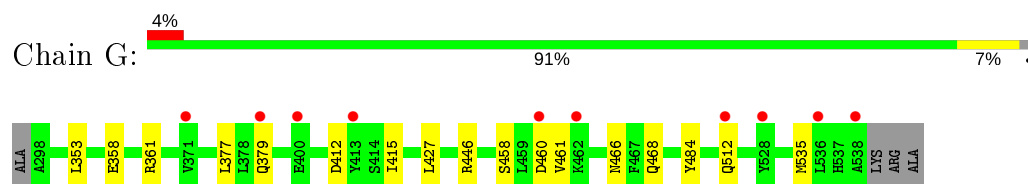
- Molecule 1: Nuclear receptor subfamily 5 group A member 2



- Molecule 1: Nuclear receptor subfamily 5 group A member 2



- Molecule 1: Nuclear receptor subfamily 5 group A member 2



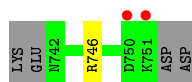
- Molecule 2: Nuclear receptor coactivator 2

Chain B:  57% 7% 36%



- Molecule 2: Nuclear receptor coactivator 2

Chain D:  14% 64% 7% 29%



- Molecule 2: Nuclear receptor coactivator 2

Chain F:  7% 50% 21% 29%



- Molecule 2: Nuclear receptor coactivator 2

Chain H:  7% 64% 7% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.95Å 76.89Å 108.48Å 90.00° 95.46° 90.00°	Depositor
Resolution (Å)	46.62 – 1.75 49.92 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.2 (46.62-1.75) 88.5 (49.92-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.214 , 0.236 0.217 , 0.239	Depositor DCC
R_{free} test set	2000 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9019	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2876e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: CPS, EPH

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	0.26	0/1989	0.42	0/2687
1	C	0.23	0/1983	0.37	0/2676
1	E	0.25	0/1997	0.41	0/2697
1	G	0.27	0/1997	0.40	0/2697
2	B	0.19	0/76	0.26	0/102
2	D	0.23	0/85	0.32	0/113
2	F	0.24	0/85	0.34	0/113
2	H	0.24	0/85	0.33	0/113
All	All	0.25	0/8297	0.40	0/11198

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	1953	0	1962	17	0
1	C	1945	0	1959	14	1
1	E	1958	0	1971	18	1
1	G	1958	0	1971	11	0
2	B	76	0	80	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	85	0	93	2	0
2	F	85	0	93	3	0
2	H	85	0	93	1	0
3	A	47	0	61	3	0
3	C	47	0	61	2	0
3	E	47	0	61	2	0
3	G	47	0	61	0	0
4	A	75	0	103	0	0
4	C	49	0	69	0	0
4	E	128	0	178	0	0
4	G	53	0	71	0	0
5	A	90	0	0	3	0
5	C	103	0	0	1	0
5	D	1	0	0	0	0
5	E	94	0	0	0	0
5	G	92	0	0	0	0
5	H	1	0	0	0	0
All	All	9019	0	8887	61	1

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 3.

All (61) 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:G:379:GLN:HE22	2:H:742:ASN:HD22	1.37	0.73
1:C:372:ASP:OD2	2:D:746:ARG:NH2	2.23	0.69
1:C:529:ASN:HD21	2:F:747:TYR:HA	1.57	0.69
1:C:493:THR:HG23	1:C:494:GLU:HG3	1.74	0.68
1:A:358:GLU:OE1	1:A:361:ARG:NH2	2.16	0.67
1:G:358:GLU:OE1	1:G:361:ARG:NH2	2.31	0.63
1:C:528:TYR:OH	2:F:746:ARG:NH1	2.32	0.62
1:E:377:LEU:HD23	1:E:461:VAL:HG21	1.82	0.61
1:A:530:ASN:O	1:A:533:ILE:N	2.34	0.60
1:C:528:TYR:HE2	2:F:750:ASP:OD2	1.86	0.59
1:A:412:ASP:HB2	1:A:415:ILE:HD13	1.83	0.58
1:E:333:ARG:HB3	1:E:337:GLU:HG3	1.85	0.58
1:C:459:LEU:HG	1:C:474:GLN:HG3	1.84	0.58
1:A:361:ARG:NH1	2:B:748:LEU:O	2.37	0.57
1:E:412:ASP:OD2	1:E:414:SER:OG	2.22	0.57
1:A:426:ASN:O	1:A:430:HIS:HD2	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:O	1:A:535:MET:HG2	2.07	0.55
1:E:528:TYR:HD1	1:E:528:TYR:H	1.55	0.54
1:E:399:LYS:HG3	1:E:410:GLN:HE22	1.72	0.54
1:G:458:SER:OG	1:G:460:ASP:OD1	2.25	0.54
1:E:399:LYS:HG3	1:E:410:GLN:NE2	2.25	0.52
1:G:468:GLN:H	1:G:468:GLN:CD	2.13	0.52
1:A:386:LEU:HD13	3:A:601:EPH:H311	1.92	0.51
1:E:531:LEU:O	1:E:535:MET:HG2	2.11	0.50
1:G:377:LEU:HD23	1:G:461:VAL:HG21	1.94	0.50
1:G:353:LEU:HD21	1:G:535:MET:HG3	1.92	0.49
1:A:350:ASP:HB2	1:A:530:ASN:OD1	2.12	0.49
1:A:426:ASN:O	1:A:430:HIS:CD2	2.67	0.48
1:A:523:ASN:OD1	5:A:701:HOH:O	2.19	0.48
1:G:446:ARG:HD2	1:G:484:TYR:OH	2.14	0.48
1:A:369:LEU:HD21	1:A:469:LEU:HD22	1.95	0.47
1:A:426:ASN:OD1	1:A:512:GLN:NE2	2.46	0.47
5:A:701:HOH:O	1:G:458:SER:OG	2.20	0.47
1:E:446:ARG:HD2	1:E:484:TYR:CE1	2.49	0.47
1:G:427:LEU:HD21	1:G:512:GLN:HG2	1.97	0.46
1:A:513:ALA:HB1	3:A:601:EPH:H141	1.97	0.46
1:E:448:PHE:CZ	1:E:452:LYS:HD2	2.50	0.46
1:E:323[B]:MET:HG2	1:E:407:THR:HB	1.99	0.45
1:G:466:ASN:HA	1:G:468:GLN:OE1	2.16	0.45
2:D:746:ARG:HE	1:E:529:ASN:ND2	2.14	0.45
1:E:513:ALA:HB1	3:E:601:EPH:H141	1.99	0.45
1:A:426:ASN:ND2	1:A:430:HIS:NE2	2.66	0.44
1:E:369:LEU:HD21	1:E:469:LEU:HD22	1.99	0.44
1:E:394:GLN:O	1:E:439:ARG:NH2	2.51	0.43
1:E:386:LEU:HB3	3:E:601:EPH:H312	1.99	0.43
1:C:531:LEU:O	1:C:535:MET:HG2	2.19	0.42
1:C:427:LEU:HD21	1:C:513:ALA:HA	2.02	0.42
1:C:459:LEU:HD21	1:C:471:GLU:HA	2.02	0.41
1:E:348:MET:HE1	1:E:405:LEU:HD13	2.02	0.41
1:A:416:ILE:HA	3:A:601:EPH:O4	2.20	0.41
3:C:601:EPH:H52	3:C:601:EPH:H221	2.03	0.41
1:C:386:LEU:HB3	3:C:601:EPH:H311	2.03	0.41
1:C:350:ASP:HA	1:C:532:LEU:HD13	2.03	0.41
1:G:412:ASP:HB3	1:G:415:ILE:HG13	2.01	0.41
1:E:446:ARG:HD2	1:E:484:TYR:CZ	2.56	0.40
1:C:370:LYS:HG2	5:C:701:HOH:O	2.21	0.40
1:C:373:ASP:OD2	1:C:465:GLU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LEU:HD23	1:A:461:VAL:HG21	2.02	0.40
1:E:399:LYS:NZ	1:E:410:GLN:HE22	2.19	0.40
1:C:359:TRP:CH2	1:C:452:LYS:HG2	2.57	0.40
1:A:298:ALA:N	5:A:710:HOH:O	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:SER:OG	1:E:412:ASP:OD1[1_565]	2.17	0.03

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	239/245 (98%)	234 (98%)	4 (2%)	1 (0%)	34	17
1	C	236/245 (96%)	232 (98%)	4 (2%)	0	100	100
1	E	240/245 (98%)	237 (99%)	1 (0%)	2 (1%)	19	6
1	G	240/245 (98%)	237 (99%)	3 (1%)	0	100	100
2	B	7/14 (50%)	7 (100%)	0	0	100	100
2	D	8/14 (57%)	8 (100%)	0	0	100	100
2	F	8/14 (57%)	8 (100%)	0	0	100	100
2	H	8/14 (57%)	8 (100%)	0	0	100	100
All	All	986/1036 (95%)	971 (98%)	12 (1%)	3 (0%)	41	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	529	ASN

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Mol	Chain	Res	Type
1	E	528	TYR
1	E	529	ASN

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	216/218 (99%)	216 (100%)	0	100	100
1	C	216/218 (99%)	216 (100%)	0	100	100
1	E	217/218 (100%)	214 (99%)	3 (1%)	67	52
1	G	217/218 (100%)	217 (100%)	0	100	100
2	B	8/13 (62%)	8 (100%)	0	100	100
2	D	9/13 (69%)	9 (100%)	0	100	100
2	F	9/13 (69%)	9 (100%)	0	100	100
2	H	9/13 (69%)	9 (100%)	0	100	100
All	All	901/924 (98%)	898 (100%)	3 (0%)	92	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	400	GLU
1	E	528	TYR
1	E	529	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	529	ASN
1	E	410	GLN
1	E	529	ASN
2	H	742	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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	CPS	C	603	-	26,27,45	0.20	0	41,44,70	0.39	0
3	EPH	E	601	-	46,46,48	0.27	0	49,51,53	0.55	0
4	CPS	E	603	-	34,34,45	0.18	0	52,53,70	0.32	0
3	EPH	C	601	-	46,46,48	0.28	0	49,51,53	0.53	0
4	CPS	G	603	-	26,26,45	0.21	0	40,43,70	0.33	0
3	EPH	A	601	-	46,46,48	0.28	0	49,51,53	0.55	0
4	CPS	C	602	-	28,28,45	0.20	0	46,46,70	0.39	0
4	CPS	G	602	-	33,33,45	0.14	0	52,52,70	0.32	0
4	CPS	A	602	-	26,27,45	0.20	0	41,44,70	0.38	0
4	CPS	E	606	-	26,27,45	0.18	0	41,44,70	0.35	0
4	CPS	E	605	-	26,26,45	0.20	0	40,43,70	0.31	0
4	CPS	E	602	-	29,29,45	0.17	0	47,47,70	0.37	0
4	CPS	E	604	-	26,27,45	0.18	0	41,44,70	0.34	0
4	CPS	A	604	-	32,32,45	0.16	0	51,51,70	0.32	0
4	CPS	A	603	-	25,25,45	0.25	0	37,41,70	0.33	0
3	EPH	G	601	-	46,46,48	0.28	0	49,51,53	0.55	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
4	CPS	C	603	-	-	0/2/67/90	0/4/4/4
3	EPH	E	601	-	-	8/50/50/52	-
4	CPS	E	603	-	-	0/12/77/90	0/4/4/4
3	EPH	C	601	-	-	9/50/50/52	-
4	CPS	G	603	-	-	-	0/4/4/4
3	EPH	A	601	-	-	8/50/50/52	-
4	CPS	C	602	-	-	0/4/69/90	0/4/4/4
4	CPS	G	602	-	-	0/11/76/90	0/4/4/4
4	CPS	A	602	-	-	0/2/67/90	0/4/4/4
4	CPS	E	606	-	-	0/2/67/90	0/4/4/4
4	CPS	E	605	-	-	-	0/4/4/4
4	CPS	E	602	-	-	0/6/71/90	0/4/4/4
4	CPS	E	604	-	-	0/2/67/90	0/4/4/4
4	CPS	A	604	-	-	0/9/74/90	0/4/4/4
4	CPS	A	603	-	-	-	0/4/4/4
3	EPH	G	601	-	-	7/50/50/52	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	EPH	C25-C26-C27-C28
3	E	601	EPH	C6-C7-C8-C9
3	G	601	EPH	C6-C7-C8-C9
3	C	601	EPH	C6-C7-C8-C9
3	A	601	EPH	C6-C7-C8-C9
3	E	601	EPH	C37-O5-P1-O8
3	C	601	EPH	C12-C13-C14-C15
3	A	601	EPH	C12-C13-C14-C15
3	E	601	EPH	C11-C10-C9-C8
3	G	601	EPH	C11-C10-C9-C8
3	G	601	EPH	C5-C6-C7-C8
3	C	601	EPH	C22-C23-C24-C25
3	C	601	EPH	C28-C29-C30-C31

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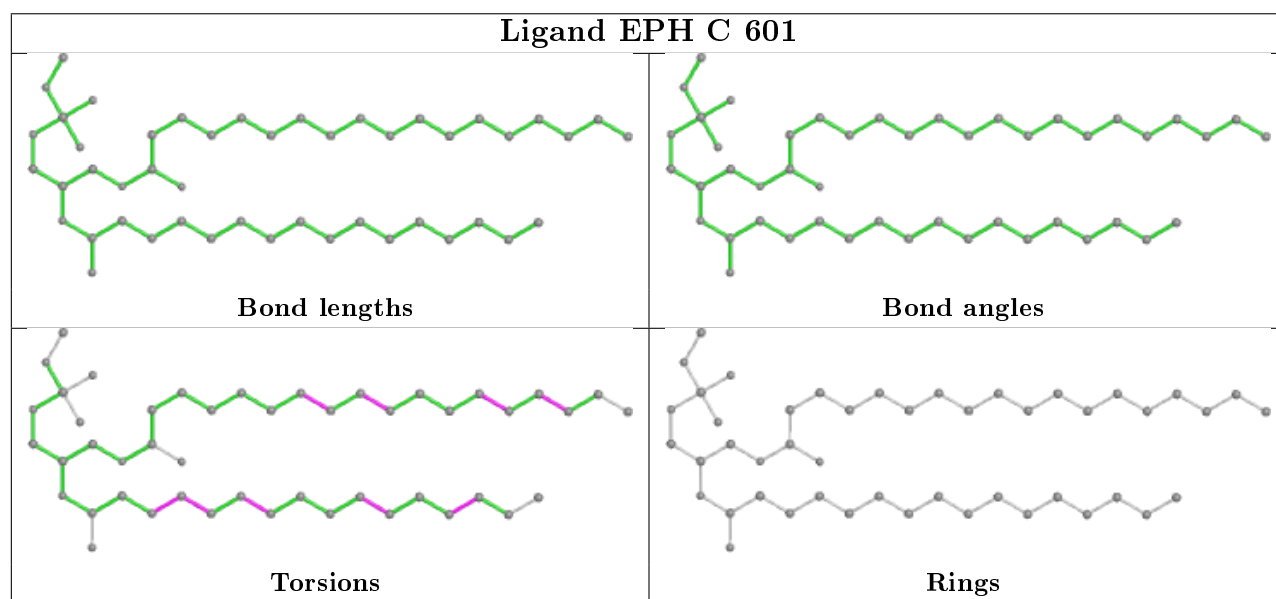
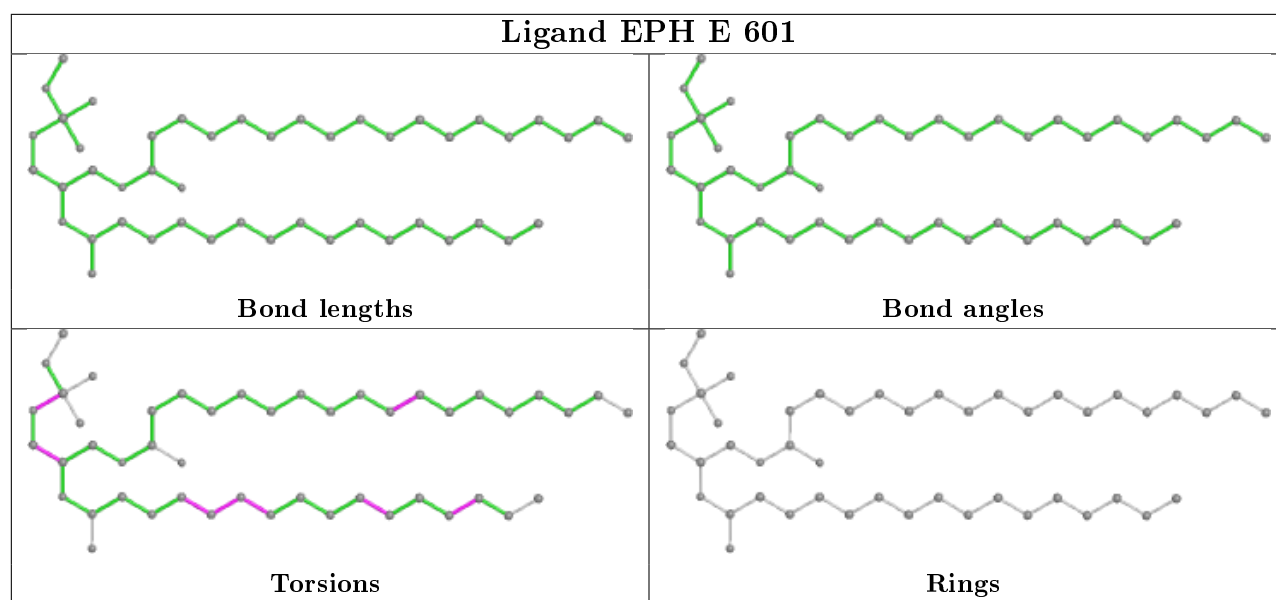
Mol	Chain	Res	Type	Atoms
3	E	601	EPH	O1-C2-C37-O5
3	G	601	EPH	C15-C16-C17-C35
3	A	601	EPH	C11-C10-C9-C8
3	A	601	EPH	C22-C23-C24-C25
3	E	601	EPH	C12-C13-C14-C15
3	G	601	EPH	C12-C13-C14-C15
3	C	601	EPH	C24-C25-C26-C27
3	A	601	EPH	C28-C29-C30-C31
3	A	601	EPH	C15-C16-C17-C35
3	C	601	EPH	C11-C10-C9-C8
3	C	601	EPH	C15-C16-C17-C35
3	C	601	EPH	C5-C6-C7-C8
3	G	601	EPH	C20-C21-C22-C23
3	C	601	EPH	C30-C31-C32-C33
3	A	601	EPH	C30-C31-C32-C33
3	G	601	EPH	C21-C22-C23-C24
3	E	601	EPH	C7-C8-C9-C10
3	A	601	EPH	C24-C25-C26-C27
3	E	601	EPH	C15-C16-C17-C35

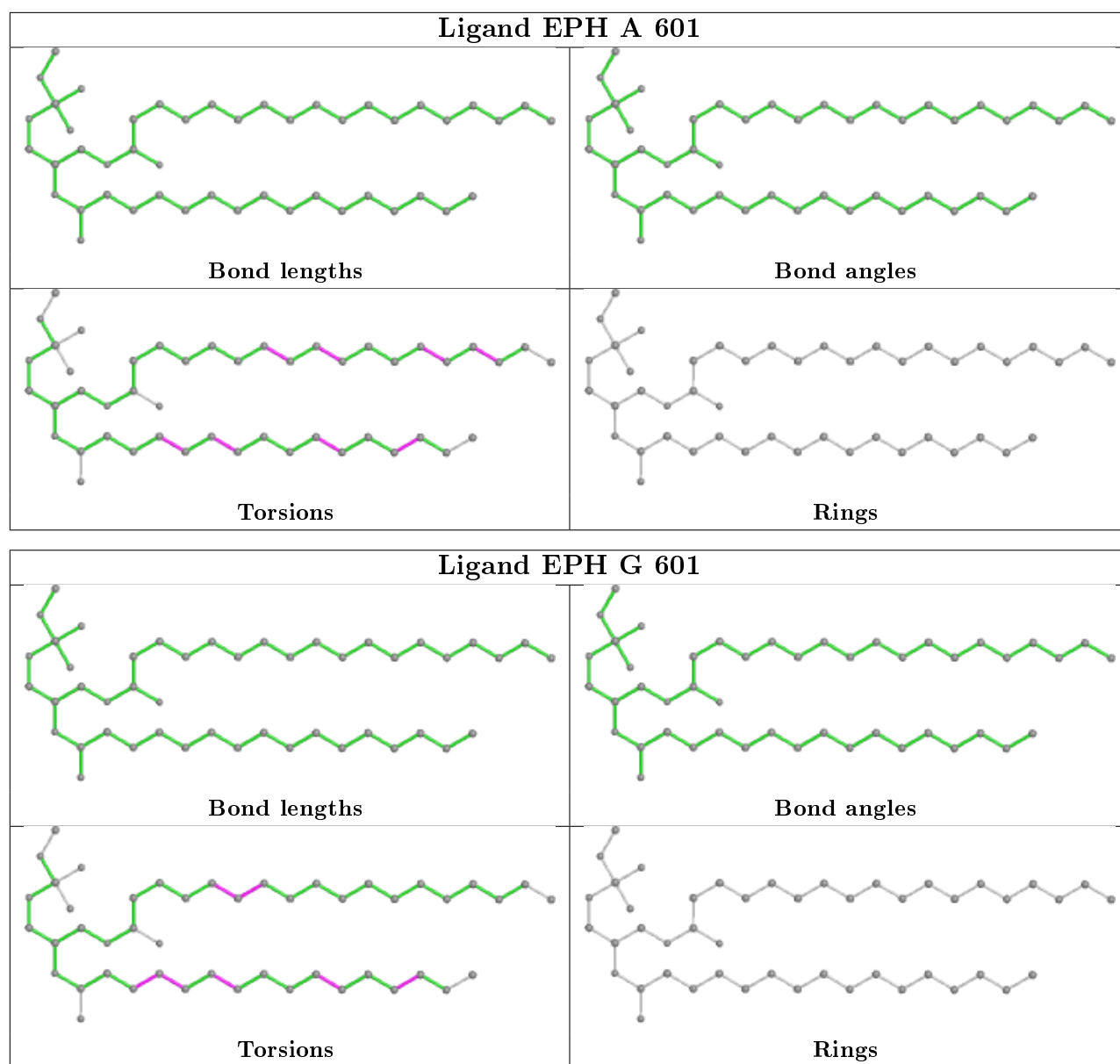
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	EPH	2	0
3	C	601	EPH	2	0
3	A	601	EPH	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	241/245 (98%)	0.63	22 (9%) 9 11	15, 29, 55, 92	0
1	C	239/245 (97%)	0.45	10 (4%) 36 42	14, 27, 50, 76	0
1	E	241/245 (98%)	0.51	14 (5%) 23 28	15, 28, 51, 88	0
1	G	241/245 (98%)	0.45	10 (4%) 37 44	15, 27, 49, 66	0
2	B	9/14 (64%)	0.50	0 100 100	31, 36, 42, 58	0
2	D	10/14 (71%)	1.21	2 (20%) 1 1	33, 38, 74, 82	0
2	F	10/14 (71%)	0.93	1 (10%) 7 9	34, 43, 66, 70	0
2	H	10/14 (71%)	0.87	1 (10%) 7 9	32, 42, 62, 65	0
All	All	1001/1036 (96%)	0.52	60 (5%) 21 27	14, 29, 53, 92	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	TYR	10.0
1	E	528	TYR	6.9
1	A	460	ASP	6.9
1	C	528	TYR	6.5
1	E	413	TYR	5.5
1	A	368	GLU	5.3
1	A	467	PHE	4.8
1	A	365	PHE	4.6
1	E	461	VAL	4.5
1	G	528	TYR	4.3
1	G	460	ASP	4.3
1	A	463	ASN	4.3
1	E	460	ASP	4.1
1	E	297	ALA	3.9
1	G	413	TYR	3.9
1	C	467	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	491	GLN	3.6
1	E	298	ALA	3.6
1	E	529	ASN	3.6
2	F	750	ASP	3.4
1	G	400	GLU	3.4
1	A	530	ASN	3.3
1	A	531	LEU	3.3
1	A	400	GLU	3.1
1	A	459	LEU	3.1
1	C	491	GLN	3.0
1	E	536	LEU	2.9
1	E	415	ILE	2.9
2	H	747	TYR	2.9
1	C	400	GLU	2.8
2	D	750	ASP	2.8
1	A	415	ILE	2.7
1	E	537	HIS	2.6
1	A	427	LEU	2.6
1	G	538	ALA	2.6
1	C	419	GLN	2.6
1	C	469	LEU	2.6
1	C	527	PRO	2.5
1	E	462	LYS	2.5
1	C	529	ASN	2.5
1	G	512	GLN	2.4
1	A	370	LYS	2.4
1	A	532	LEU	2.4
1	A	462	LYS	2.3
1	A	527	PRO	2.3
2	D	751	LYS	2.3
1	A	369	LEU	2.2
1	A	461	VAL	2.2
1	G	371	VAL	2.2
1	G	462	LYS	2.2
1	A	419	GLN	2.1
1	E	530	ASN	2.1
1	C	530	ASN	2.1
1	G	536	LEU	2.1
1	G	379	GLN	2.1
1	A	413	TYR	2.1
1	E	368	GLU	2.1
1	E	534	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	361	ARG	2.0
1	C	465	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

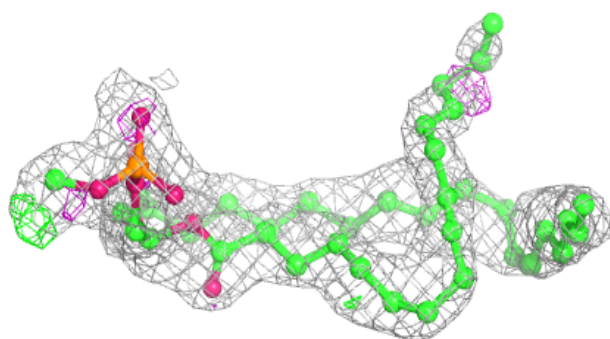
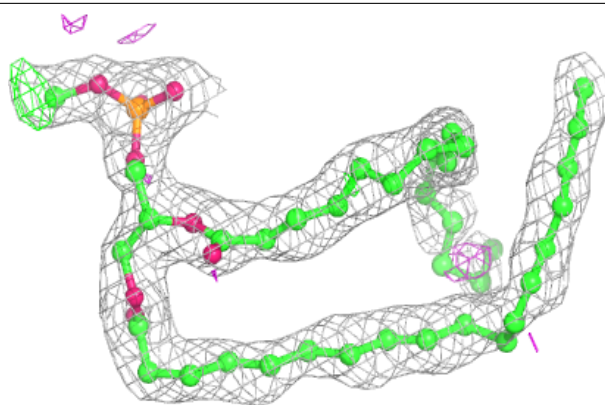
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CPS	E	606	24/42	0.75	0.15	34,39,42,44	0
4	CPS	C	603	24/42	0.77	0.16	32,36,44,47	0
4	CPS	E	603	31/42	0.81	0.17	20,26,43,45	0
4	CPS	A	603	22/42	0.82	0.14	30,34,39,45	0
4	CPS	E	604	24/42	0.84	0.13	27,30,35,38	0
4	CPS	A	604	29/42	0.86	0.13	25,29,42,45	0
4	CPS	G	603	23/42	0.86	0.13	28,31,35,39	0
4	CPS	E	602	26/42	0.87	0.13	21,24,34,36	0
4	CPS	A	602	24/42	0.88	0.11	28,33,37,37	0
3	EPH	C	601	47/49	0.88	0.17	26,37,46,48	0
4	CPS	G	602	30/42	0.89	0.11	19,25,40,46	0
3	EPH	E	601	47/49	0.89	0.16	29,41,54,57	0
4	CPS	C	602	25/42	0.89	0.11	25,30,37,38	0
4	CPS	E	605	23/42	0.89	0.12	25,29,31,32	0
3	EPH	A	601	47/49	0.90	0.15	31,41,50,53	0
3	EPH	G	601	47/49	0.92	0.16	23,35,54,58	0

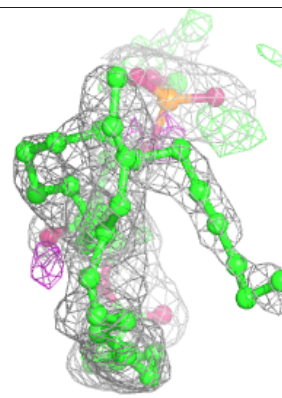
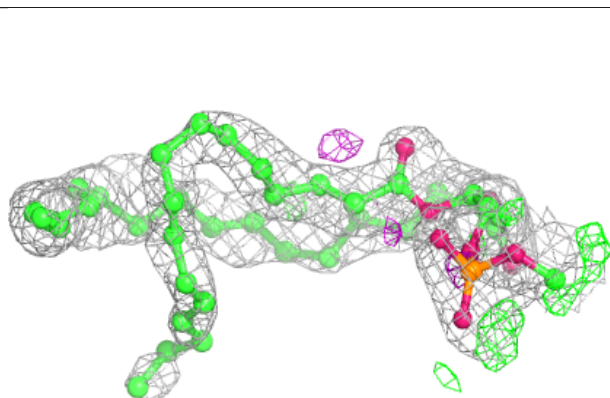
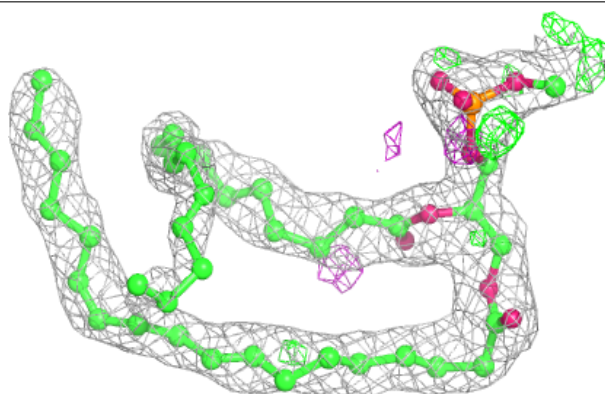
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EPH C 601:

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

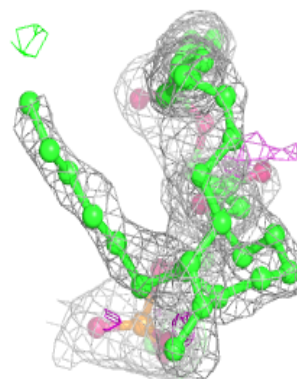
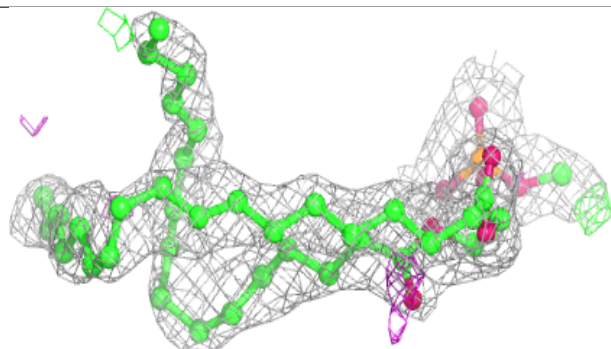
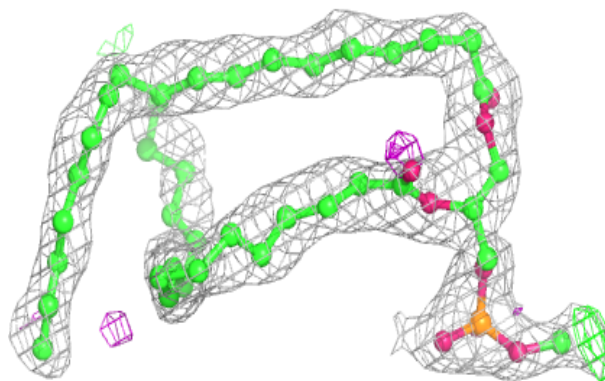
**Electron density around EPH E 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

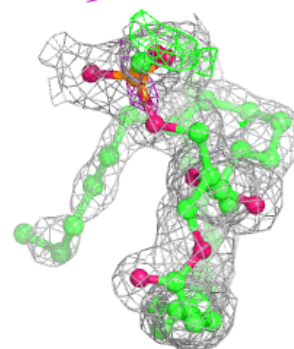
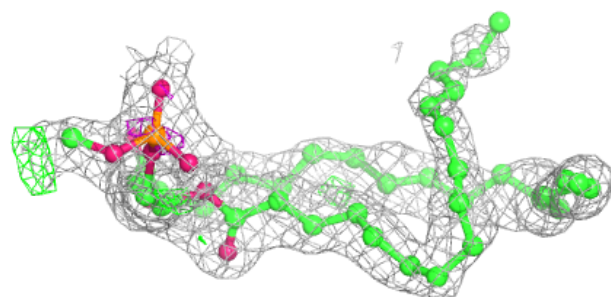
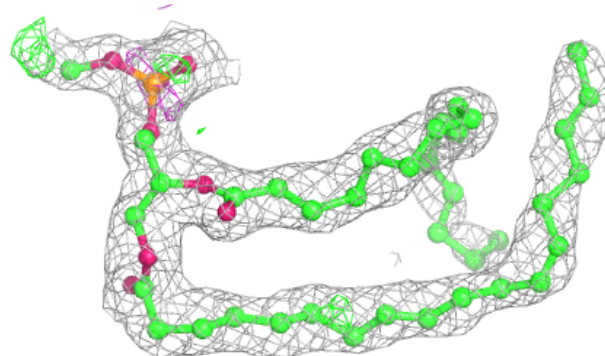


Electron density around EPH A 601:

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

**Electron density around EPH G 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.