Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2021 – 12:11 pm BST

PDB ID	:	7BJV
Title	:	Crystal structure of the ligand-binding domains of the heterodimer EcR/USP bound to the synthetic agonist BYI09181
Authors	:	Browning, C.; McEwen, A.G.; Billas, I.M.L.
Deposited on	:	2021-01-14
Resolution	:	3.05 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:

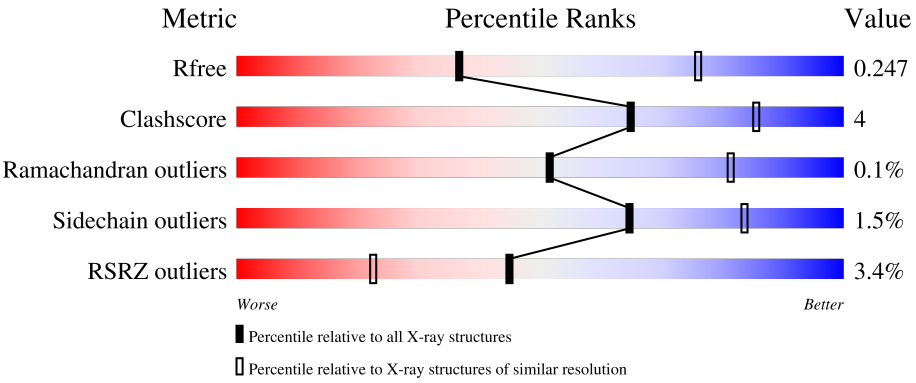
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 <=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	263	2% 83% 11% • 5%
1	B	263	3% 84% 10% • 6%
1	C	263	2% 87% 8% • •
2	D	266	5% 79% 11% 10%
2	E	266	3% 76% 8% 16%

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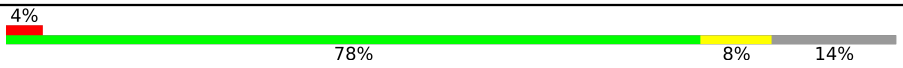
Mol	Chain	Length	Quality of chain
2	F	266	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11762 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 Ultraspiracle protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	1	0
			1991	1274	347	357	13			
1	B	247	Total	C	N	O	S	0	0	0
			1959	1257	344	346	12			
1	C	252	Total	C	N	O	S	0	0	0
			1997	1276	350	359	12			

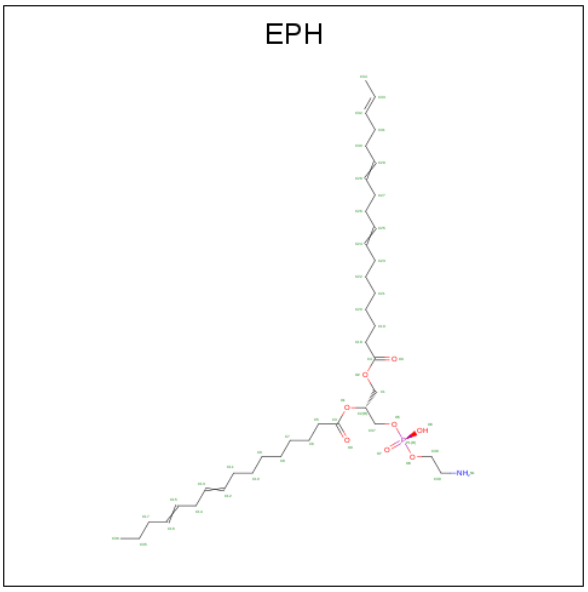
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	MET	-	initiating methionine	UNP A0A2A4K9Z3
B	204	MET	-	initiating methionine	UNP A0A2A4K9Z3
C	204	MET	-	initiating methionine	UNP A0A2A4K9Z3

- Molecule 2 is a protein called Ecdysone Receptor.

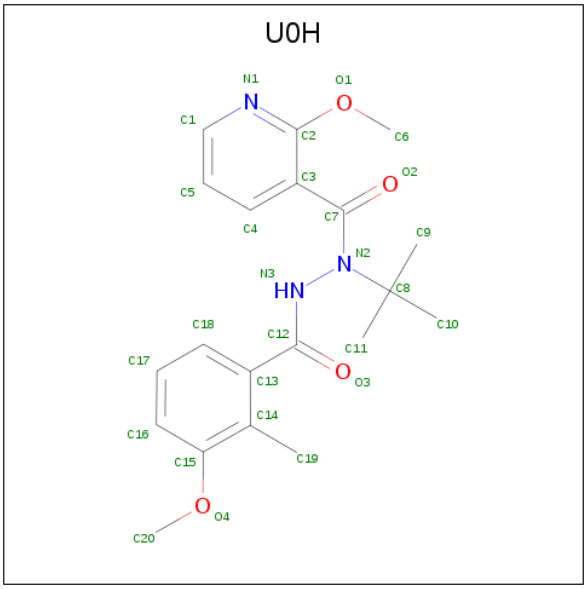
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	240	Total	C	N	O	S	0	1	0
			1880	1199	318	348	15			
2	E	223	Total	C	N	O	S	0	1	0
			1769	1134	302	318	15			
2	F	230	Total	C	N	O	S	0	2	0
			1824	1166	310	333	15			

- 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	N	O	P	0	0
			49	39	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
3	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 4 is {N}- {tert}-butyl-2-methoxy- {N}'-(3-methoxy-2-methyl-phenyl)carbonyl-pyridine-3-carbohydrazide (three-letter code: U0H) (formula: $C_{20}H_{25}N_3O_4$) (labeled as "Ligand of Interest" by depositor).

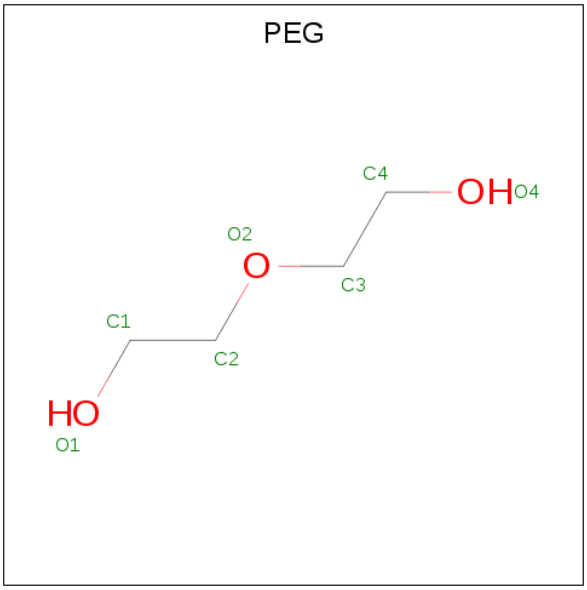


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C N O 27 20 3 4	0	0
4	E	1	Total C N O 27 20 3 4	0	0
4	F	1	Total C N O 27 20 3 4	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Mg 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

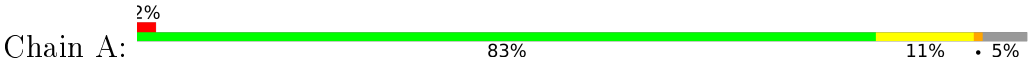
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	14	Total O 14 14	0	0
7	B	14	Total O 14 14	0	0
7	C	22	Total O 22 22	0	0
7	D	12	Total O 12 12	0	0
7	E	15	Total O 15 15	0	0
7	F	15	Total O 15 15	0	0

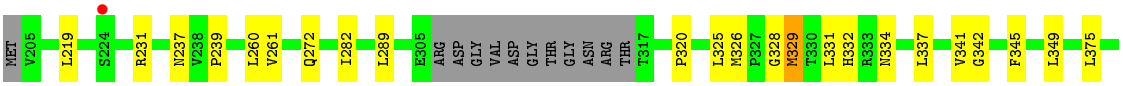
3 Residue-property plots (i)

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: Ultraspiracle protein

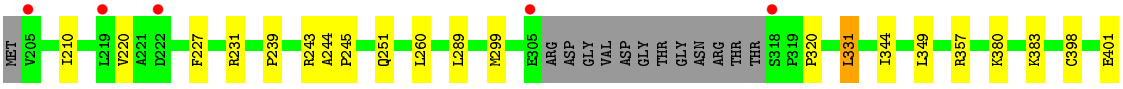
Chain A:

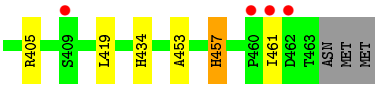




- Molecule 1: Ultraspiracle protein

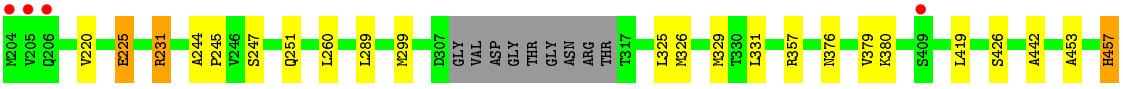
Chain B:

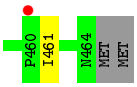




- Molecule 1: Ultraspiracle protein

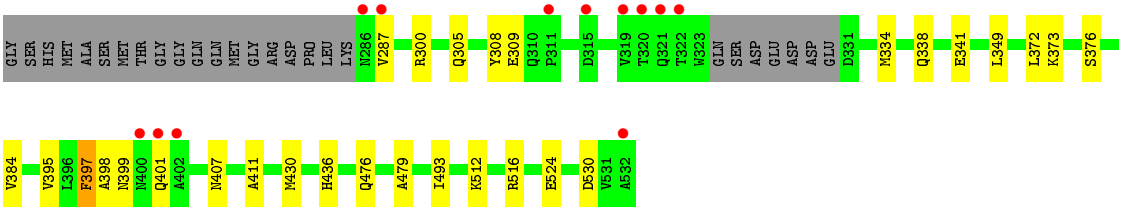
Chain C:



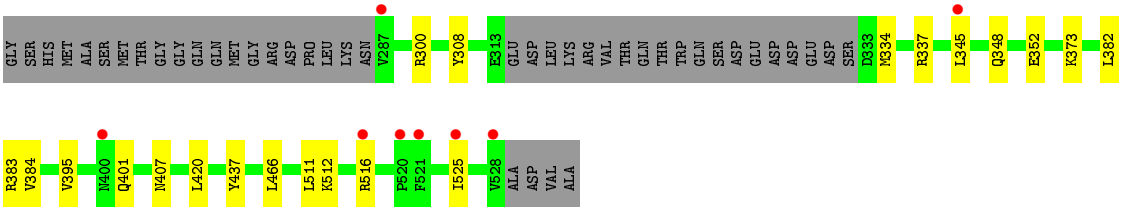


- Molecule 2: Ecdysone Receptor

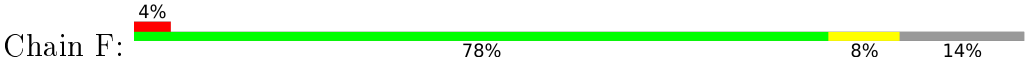
Chain D:

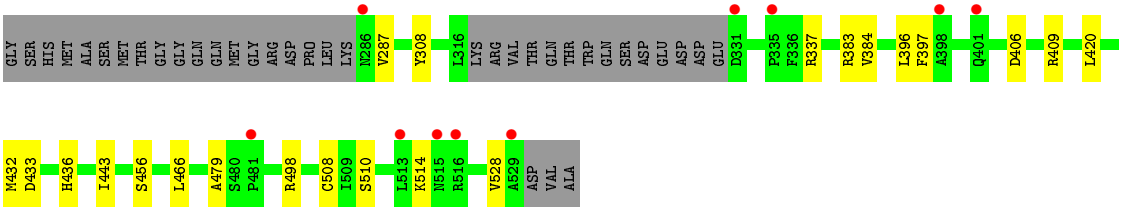


• Molecule 2: Ecdysone Receptor



• Molecule 2: Ecdysone Receptor





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.03Å 147.03Å 162.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.79 – 3.05 49.79 – 3.05	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.79-3.05) 96.0 (49.79-3.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.19 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.196 , 0.247 0.196 , 0.247	Depositor DCC
R_{free} test set	1881 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11762	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U0H, EPH, PEG, MG

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	0.24	0/2032	0.45	0/2746
1	B	0.24	0/1997	0.45	0/2699
1	C	0.24	0/2035	0.46	0/2751
2	D	0.23	0/1915	0.43	0/2595
2	E	0.23	0/1804	0.43	0/2442
2	F	0.23	0/1862	0.43	0/2521
All	All	0.24	0/11645	0.44	0/15754

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

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	1991	0	2026	25	0
1	B	1959	0	1997	15	0
1	C	1997	0	2017	15	0
2	D	1880	0	1870	15	0
2	E	1769	0	1789	13	0
2	F	1824	0	1834	12	0
3	A	49	0	67	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	49	0	67	1	0
3	C	49	0	67	3	0
4	D	27	0	0	0	0
4	E	27	0	0	0	0
4	F	27	0	0	0	0
5	D	1	0	0	0	0
6	E	7	0	10	0	0
6	F	14	0	20	0	0
7	A	14	0	0	0	0
7	B	14	0	0	0	0
7	C	22	0	0	0	0
7	D	12	0	0	0	0
7	E	15	0	0	0	0
7	F	15	0	0	1	0
All	All	11762	0	11764	95	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 (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326[B]:MET:HG2	1:A:329:MET:HB2	1.58	0.86
1:A:326[A]:MET:HG2	1:A:329:MET:HB2	1.64	0.78
2:E:334:MET:HG2	2:E:337:ARG:HB2	1.64	0.77
1:A:325:LEU:HD11	1:A:331:LEU:HD12	1.69	0.74
1:C:326:MET:HG2	1:C:329:MET:HB3	1.77	0.65
2:E:308:TYR:O	2:E:383[B]:ARG:NH2	2.32	0.62
1:C:325:LEU:HD11	1:C:331:LEU:HD12	1.81	0.62
2:D:512:LYS:HE2	2:D:530:ASP:HA	1.83	0.60
1:B:299:MET:O	1:B:357:ARG:NH1	2.35	0.60
2:F:384:VAL:HG11	2:F:420:LEU:HD21	1.83	0.59
1:C:260:LEU:HD21	1:C:289:LEU:HB2	1.84	0.58
1:B:260:LEU:HD21	1:B:289:LEU:HB2	1.85	0.58
1:A:385:ARG:NH1	1:A:389:GLU:OE2	2.37	0.57
2:E:401:GLN:O	2:E:407:ASN:ND2	2.37	0.57
2:D:397:PHE:O	2:D:399:ASN:N	2.38	0.56
1:A:325:LEU:HB2	1:A:329:MET:HB3	1.89	0.55
1:C:247:SER:O	1:C:251:GLN:NE2	2.40	0.55
2:D:308:TYR:HB3	2:D:349:LEU:HB3	1.89	0.55
2:E:511:LEU:HD22	2:E:516:ARG:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:384:VAL:HG11	2:E:420:LEU:HD21	1.90	0.54
2:E:511:LEU:HB3	2:E:516:ARG:HB2	1.91	0.53
1:C:299:MET:O	1:C:357:ARG:NH2	2.42	0.53
2:D:287:VAL:HG13	2:D:479:ALA:HB2	1.89	0.53
2:D:373:LYS:NZ	2:D:524:GLU:O	2.42	0.52
1:C:331:LEU:HD11	3:C:501:EPH:H222	1.89	0.52
1:A:261:VAL:HG22	1:A:282:ILE:HG21	1.92	0.51
1:B:210:ILE:HG13	1:B:398:CYS:HB3	1.91	0.51
1:A:345:PHE:HD2	3:A:501:EPH:H363	1.75	0.51
3:A:501:EPH:H141	3:A:501:EPH:H342	1.93	0.51
2:F:508:CYS:HB3	2:F:528:VAL:HG11	1.93	0.50
1:B:453:ALA:O	1:B:457:HIS:HB2	2.12	0.50
2:D:411:ALA:O	2:D:516:ARG:NH1	2.35	0.50
2:F:498:ARG:NH1	7:F:702:HOH:O	2.45	0.49
1:B:401:GLU:OE2	1:B:405:ARG:NH2	2.45	0.49
1:A:237:ASN:ND2	1:A:437:PHE:O	2.40	0.49
1:A:331:LEU:HD11	3:A:501:EPH:H211	1.95	0.48
1:A:453:ALA:O	1:A:457:HIS:HB2	2.13	0.47
2:E:384:VAL:HG13	2:E:395:VAL:HG11	1.96	0.47
1:A:260:LEU:HD21	1:A:289:LEU:HB2	1.96	0.47
1:A:332:HIS:HD2	1:A:334:ASN:H	1.62	0.47
2:E:373:LYS:HG2	2:E:525:ILE:HD12	1.97	0.47
1:A:341:VAL:HG11	3:A:501:EPH:H101	1.97	0.47
1:A:272:GLN:OE1	1:A:272:GLN:N	2.47	0.47
2:F:443:ILE:HD13	2:F:466:LEU:HD23	1.96	0.47
2:D:305:GLN:O	2:D:309:GLU:HG3	2.15	0.46
1:A:239:PRO:HD2	3:A:501:EPH:O3	2.16	0.46
2:F:308:TYR:O	2:F:383[B]:ARG:NH2	2.49	0.46
1:A:375:LEU:HD13	1:A:391:LEU:HB3	1.96	0.46
1:B:331:LEU:HD11	3:B:501:EPH:H212	1.97	0.45
3:C:501:EPH:H301	3:C:501:EPH:H272	1.58	0.45
2:F:287:VAL:HG13	2:F:479:ALA:HB2	1.98	0.45
1:A:337:LEU:HD23	1:A:342:GLY:HA3	1.99	0.45
2:F:432:MET:HB3	2:F:436:HIS:HB2	1.98	0.45
2:E:382:LEU:HB3	2:E:437:TYR:HE1	1.81	0.45
1:B:419:LEU:HD11	2:E:466:LEU:HD11	1.99	0.45
1:A:320:PRO:HB2	1:A:349:LEU:HD13	1.98	0.45
2:D:334:MET:HG3	2:D:338:GLN:HE21	1.82	0.45
1:A:331:LEU:HD13	3:A:501:EPH:H362	1.99	0.44
1:C:376:ASN:HB3	1:C:379:VAL:HG23	2.00	0.44
2:D:401:GLN:O	2:D:407:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HB3	1:A:460:PRO:HB2	2.00	0.44
1:C:225:GLU:H	1:C:225:GLU:HG2	1.61	0.44
2:F:406:ASP:OD1	2:F:409:ARG:NH1	2.52	0.43
2:D:308:TYR:HD1	2:D:349:LEU:HD22	1.83	0.43
1:A:430:LYS:HD2	1:A:430:LYS:HA	1.91	0.43
1:C:244:ALA:HB3	1:C:245:PRO:HD3	2.01	0.43
2:D:384:VAL:HA	2:D:397:PHE:HE1	1.82	0.43
1:B:227:PHE:HE2	1:B:457:HIS:CD2	2.36	0.43
2:F:510:SER:O	2:F:514:LYS:HD2	2.18	0.43
1:C:453:ALA:O	1:C:457:HIS:HB2	2.19	0.43
2:D:384:VAL:HG13	2:D:395:VAL:HG11	2.01	0.43
1:C:426:SER:OG	2:F:498:ARG:HD2	2.18	0.42
1:C:220:VAL:O	1:C:461:ILE:N	2.52	0.42
2:E:348:GLN:O	2:E:352:GLU:HG2	2.19	0.42
1:B:380:LYS:HE3	1:B:380:LYS:HB2	1.83	0.42
1:B:383:LYS:HE2	1:B:383:LYS:HB3	1.87	0.42
2:D:436:HIS:CE1	2:D:476:GLN:HE22	2.38	0.42
2:E:512:LYS:HE2	2:E:512:LYS:HB3	1.89	0.42
2:D:430:MET:SD	2:D:493:ILE:HD11	2.60	0.42
1:B:320:PRO:HB2	1:B:349:LEU:HD13	2.03	0.41
1:C:231:ARG:HD2	1:C:442:ALA:HB2	2.02	0.41
1:A:326[B]:MET:HG3	1:A:328:GLY:H	1.85	0.41
1:B:239:PRO:O	1:B:243:ARG:HG3	2.20	0.41
1:A:237:ASN:OD1	1:A:237:ASN:N	2.44	0.41
1:A:455:ARG:NH2	2:F:433:ASP:HB3	2.36	0.41
3:A:501:EPH:H272	3:A:501:EPH:H301	1.64	0.41
3:C:501:EPH:H211	3:C:501:EPH:H24	1.78	0.41
1:C:419:LEU:HD11	2:F:466:LEU:HD11	2.03	0.41
2:D:372:LEU:O	2:D:376:SER:OG	2.26	0.41
1:C:380:LYS:HB2	1:C:380:LYS:HE3	1.73	0.40
1:A:332:HIS:CD2	1:A:334:ASN:H	2.38	0.40
1:B:344:ILE:HD12	1:B:434:HIS:HD2	1.86	0.40
1:B:220:VAL:O	1:B:461:ILE:N	2.51	0.40
1:B:244:ALA:HB3	1:B:245:PRO:HD3	2.03	0.40
2:E:382:LEU:HB3	2:E:437:TYR:CE1	2.57	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	246/263 (94%)	242 (98%)	4 (2%)	0	100 100
1	B	243/263 (92%)	235 (97%)	8 (3%)	0	100 100
1	C	248/263 (94%)	238 (96%)	10 (4%)	0	100 100
2	D	237/266 (89%)	231 (98%)	5 (2%)	1 (0%)	34 64
2	E	220/266 (83%)	216 (98%)	4 (2%)	0	100 100
2	F	228/266 (86%)	224 (98%)	4 (2%)	0	100 100
All	All	1422/1587 (90%)	1386 (98%)	35 (2%)	1 (0%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	398	ALA

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	219/232 (94%)	216 (99%)	3 (1%)	67 84
1	B	213/232 (92%)	209 (98%)	4 (2%)	57 79
1	C	217/232 (94%)	214 (99%)	3 (1%)	67 84
2	D	202/236 (86%)	199 (98%)	3 (2%)	65 83
2	E	192/236 (81%)	190 (99%)	2 (1%)	76 89
2	F	198/236 (84%)	194 (98%)	4 (2%)	55 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1241/1404 (88%)	1222 (98%)	19 (2%)	65 83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	ARG
1	A	329	MET
1	A	457	HIS
1	B	231	ARG
1	B	251	GLN
1	B	331	LEU
1	B	457	HIS
1	C	225	GLU
1	C	231	ARG
1	C	457	HIS
2	D	300	ARG
2	D	341	GLU
2	D	397	PHE
2	E	300	ARG
2	E	345	LEU
2	F	337	ARG
2	F	396	LEU
2	F	397	PHE
2	F	456	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	332	HIS
1	A	343	GLN
1	A	386	GLN
1	B	206	GLN
1	B	434	HIS
1	B	457	HIS
1	C	287	ASN
2	D	310	GLN
2	D	338	GLN
2	D	476	GLN
2	D	477	ASN
2	E	338	GLN

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Mol	Chain	Res	Type
2	E	407	ASN
2	F	338	GLN
2	F	348	GLN
2	F	407	ASN
2	F	422	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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	EPH	C	501	-	48,48,48	0.94	2 (4%)	51,53,53	1.11	3 (5%)
6	PEG	F	603	-	6,6,6	0.43	0	5,5,5	0.30	0
3	EPH	A	501	-	48,48,48	0.93	2 (4%)	51,53,53	1.12	4 (7%)
4	U0H	D	601	-	28,28,28	0.68	1 (3%)	35,40,40	0.42	0
4	U0H	F	601	-	28,28,28	0.74	1 (3%)	35,40,40	0.42	0
6	PEG	E	602	-	6,6,6	0.45	0	5,5,5	0.28	0
6	PEG	F	602	-	6,6,6	0.44	0	5,5,5	0.31	0
3	EPH	B	501	-	48,48,48	0.94	2 (4%)	51,53,53	1.11	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	U0H	E	601	-	28,28,28	0.78	1 (3%)	35,40,40	0.42	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
3	EPH	C	501	-	-	16/52/52/52	-
6	PEG	F	603	-	-	0/4/4/4	-
3	EPH	A	501	-	-	14/52/52/52	-
4	U0H	D	601	-	-	0/26/26/26	0/2/2/2
4	U0H	F	601	-	-	1/26/26/26	0/2/2/2
6	PEG	E	602	-	-	0/4/4/4	-
6	PEG	F	602	-	-	0/4/4/4	-
3	EPH	B	501	-	-	15/52/52/52	-
4	U0H	E	601	-	-	1/26/26/26	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	EPH	O2-C4	4.30	1.45	1.33
3	C	501	EPH	O2-C4	4.30	1.45	1.33
3	A	501	EPH	O2-C4	4.25	1.45	1.33
4	E	601	U0H	C7-N2	4.06	1.40	1.35
3	C	501	EPH	O1-C3	4.04	1.45	1.34
3	B	501	EPH	O1-C3	4.02	1.45	1.34
3	A	501	EPH	O1-C3	3.97	1.45	1.34
4	F	601	U0H	C7-N2	3.85	1.40	1.35
4	D	601	U0H	C7-N2	3.57	1.40	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	EPH	O1-C3-C5	4.18	120.50	111.50
3	C	501	EPH	O1-C3-C5	4.05	120.23	111.50
3	B	501	EPH	O1-C3-C5	4.00	120.13	111.50
3	A	501	EPH	C2-O1-C3	-2.82	110.86	117.79
3	B	501	EPH	O2-C4-C18	2.67	120.29	111.91
3	C	501	EPH	O2-C4-C18	2.59	120.03	111.91
3	B	501	EPH	C2-O1-C3	-2.56	111.50	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	EPH	O2-C4-C18	2.46	119.61	111.91
3	C	501	EPH	C2-O1-C3	-2.30	112.13	117.79
3	A	501	EPH	O1-C3-O3	-2.13	118.56	123.70

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	EPH	C37-O5-P1-O7
3	A	501	EPH	C12-C13-C14-C15
3	A	501	EPH	C38-O8-P1-O7
3	B	501	EPH	C13-C14-C15-C16
3	B	501	EPH	C16-C17-C35-C36
3	B	501	EPH	O8-C38-C39-N1
3	C	501	EPH	C25-C26-C27-C28
3	C	501	EPH	C29-C30-C31-C32
3	C	501	EPH	C37-O5-P1-O6
3	C	501	EPH	C37-O5-P1-O7
3	C	501	EPH	C37-O5-P1-O8
3	C	501	EPH	C38-O8-P1-O6
3	C	501	EPH	C38-O8-P1-O7
3	C	501	EPH	C3-C5-C6-C7
3	A	501	EPH	C37-O5-P1-O8
3	C	501	EPH	C38-O8-P1-O5
3	B	501	EPH	C11-C10-C9-C8
3	C	501	EPH	C7-C8-C9-C10
3	C	501	EPH	C16-C17-C35-C36
3	A	501	EPH	C5-C6-C7-C8
3	A	501	EPH	C21-C22-C23-C24
3	B	501	EPH	C1-C2-C37-O5
3	C	501	EPH	C12-C13-C14-C15
3	B	501	EPH	O1-C2-C37-O5
3	B	501	EPH	C19-C20-C21-C22
3	B	501	EPH	C29-C30-C31-C32
3	C	501	EPH	C21-C22-C23-C24
3	B	501	EPH	C7-C8-C9-C10
3	A	501	EPH	C19-C20-C21-C22
3	A	501	EPH	C38-O8-P1-O5
3	A	501	EPH	C37-O5-P1-O6
3	A	501	EPH	C38-O8-P1-O6
3	A	501	EPH	O8-C38-C39-N1
4	E	601	U0H	C4-C3-C7-N2

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Mol	Chain	Res	Type	Atoms
3	B	501	EPH	C5-C6-C7-C8
3	A	501	EPH	C22-C23-C24-C25
3	C	501	EPH	C22-C23-C24-C25
3	B	501	EPH	C15-C16-C17-C35
3	B	501	EPH	C25-C26-C27-C28
3	A	501	EPH	C10-C11-C12-C13
4	F	601	U0H	N3-C12-C13-C18
3	A	501	EPH	C24-C25-C26-C27
3	B	501	EPH	C28-C29-C30-C31
3	C	501	EPH	C24-C25-C26-C27
3	B	501	EPH	C10-C11-C12-C13
3	C	501	EPH	O1-C3-C5-C6
3	B	501	EPH	C22-C23-C24-C25

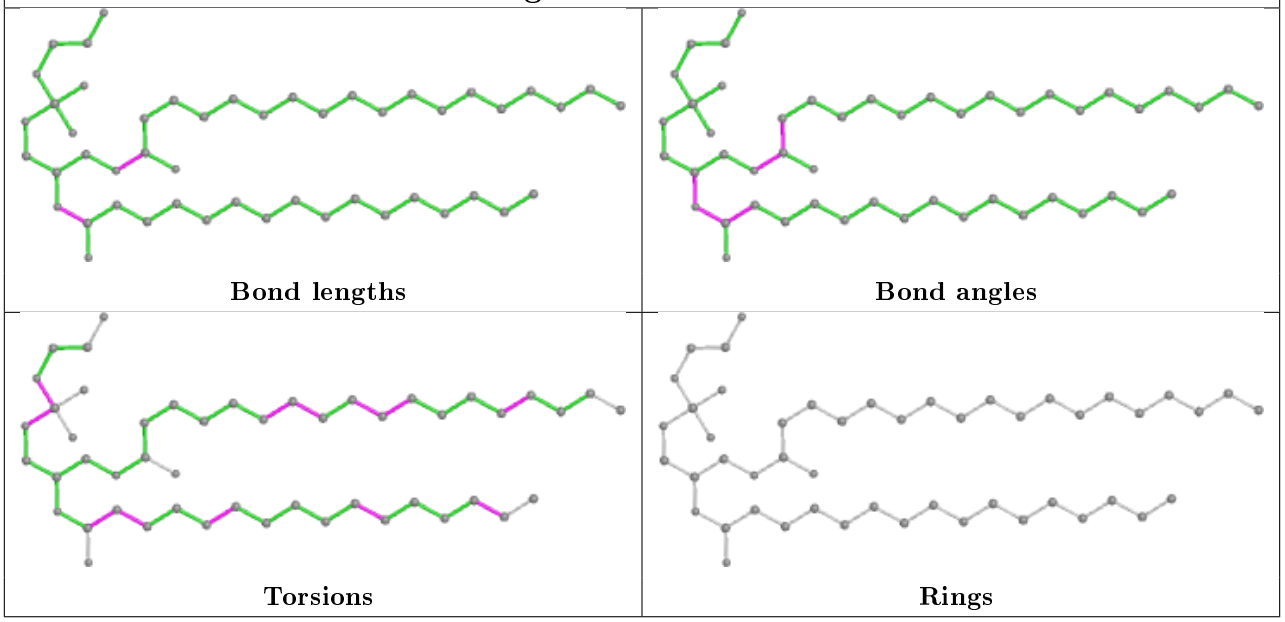
There are no ring outliers.

3 monomers are involved in 11 short contacts:

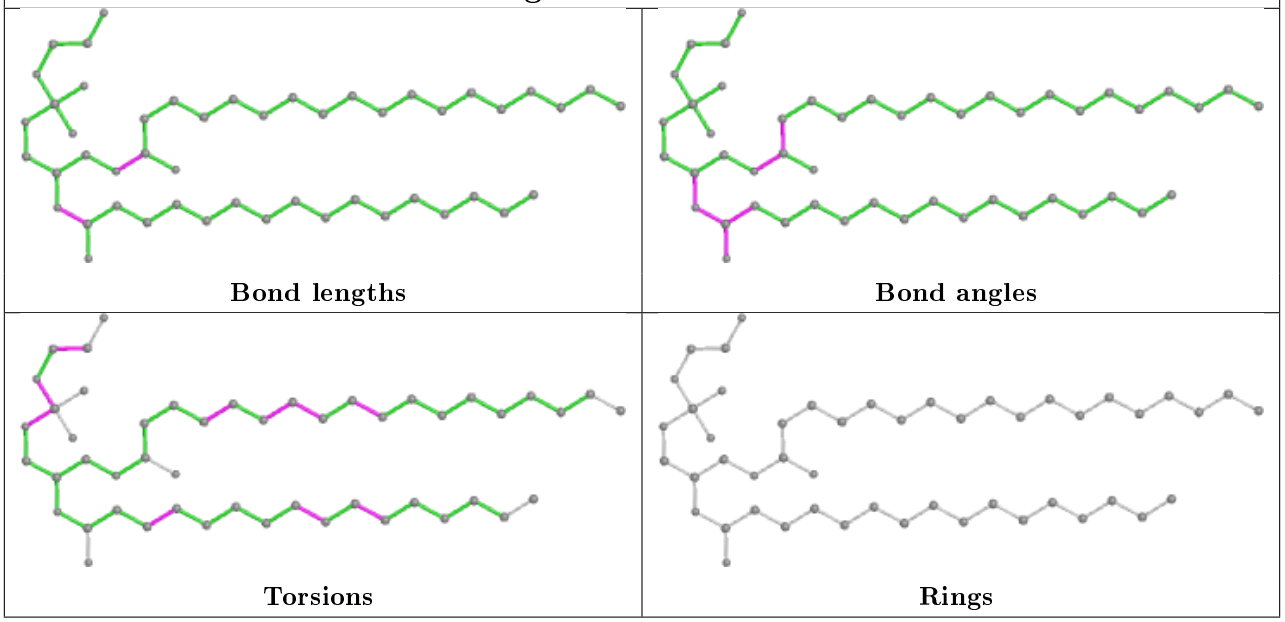
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	EPH	3	0
3	A	501	EPH	7	0
3	B	501	EPH	1	0

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 then 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.

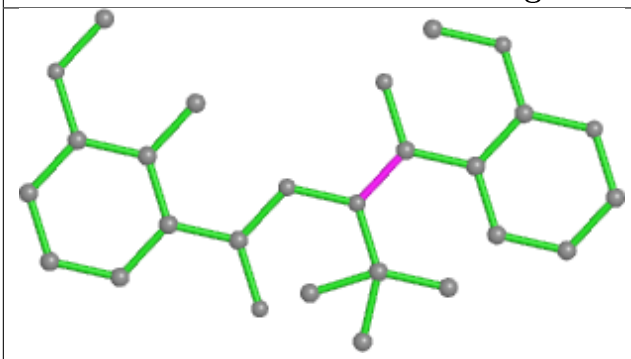
Ligand EPH C 501



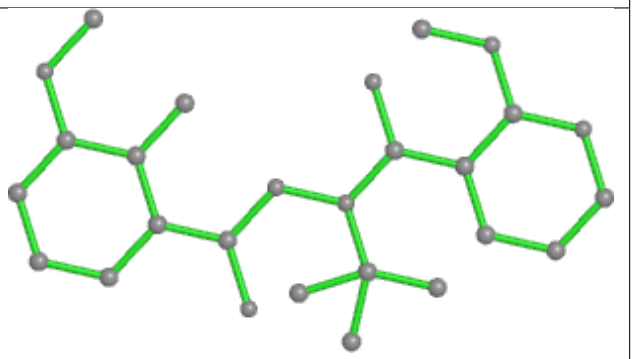
Ligand EPH A 501



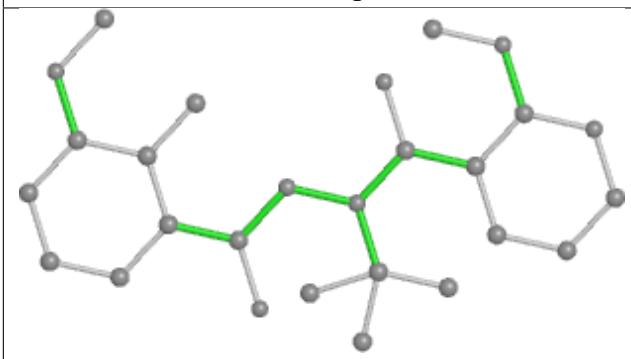
Ligand U0H D 601



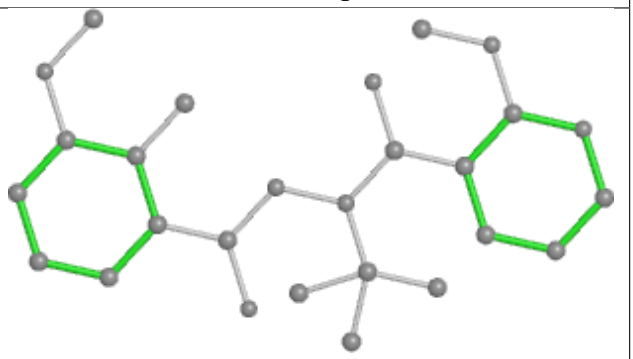
Bond lengths



Bond angles

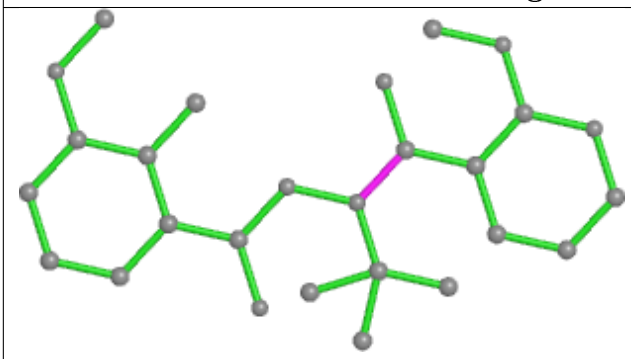


Torsions

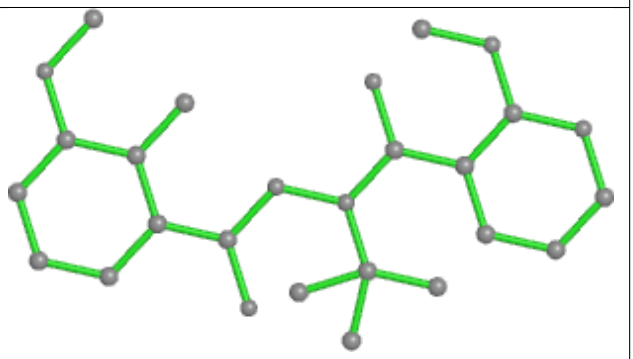


Rings

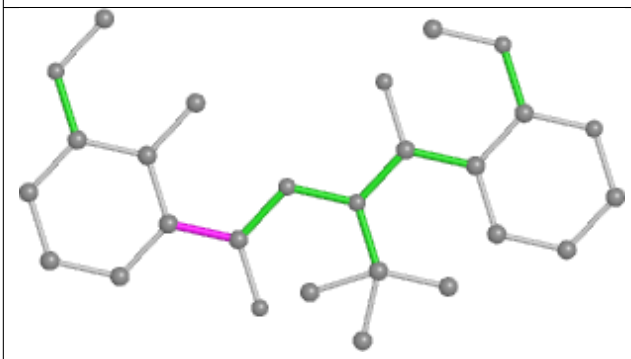
Ligand U0H F 601



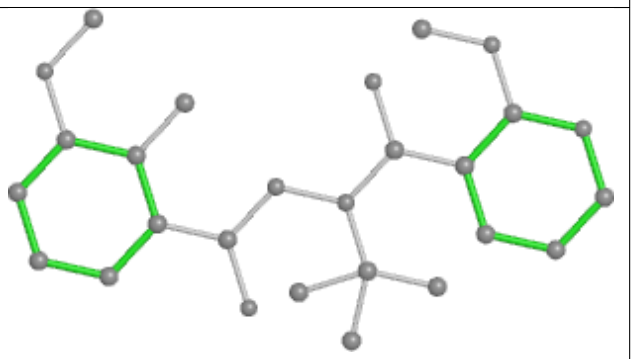
Bond lengths



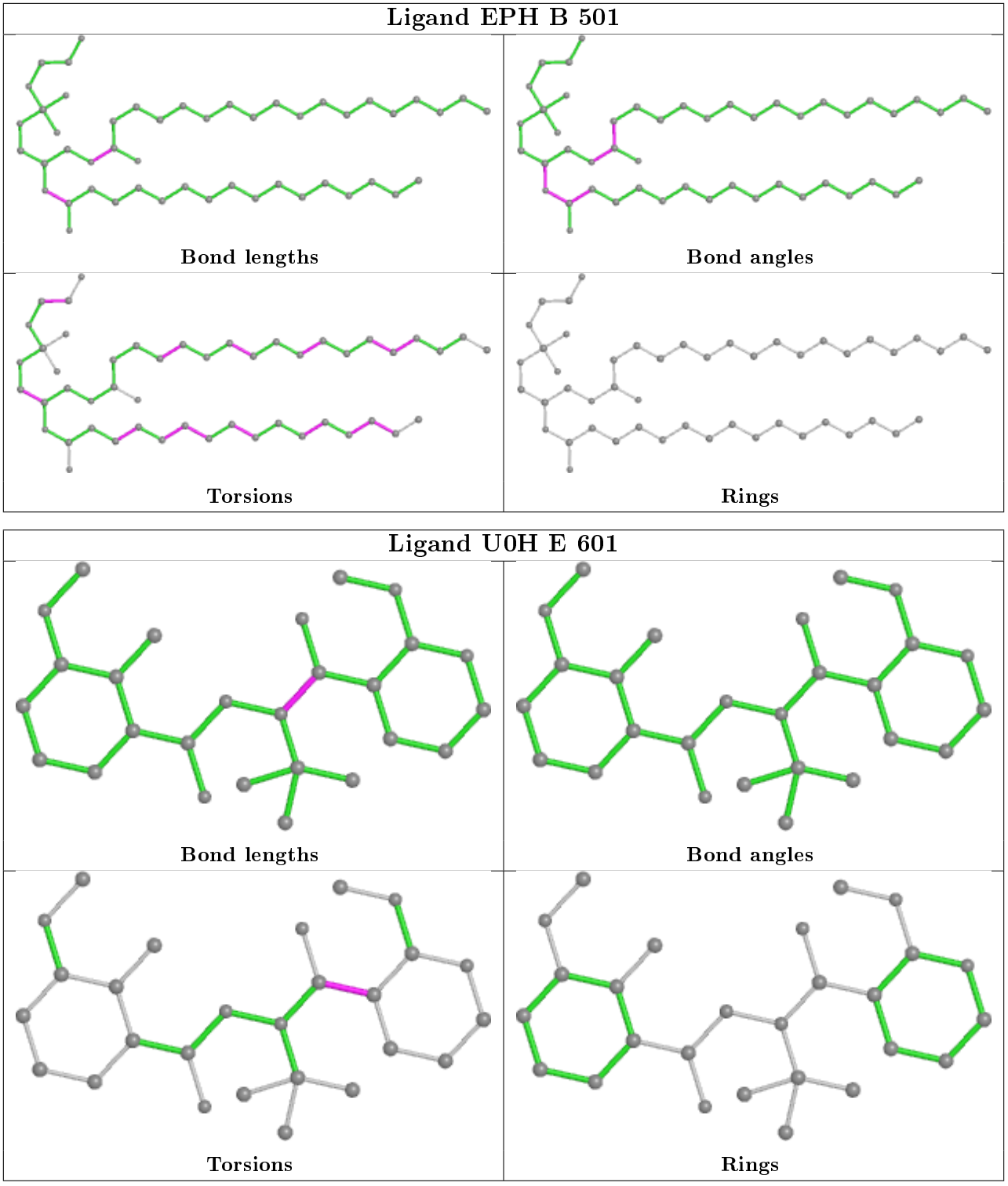
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	249/263 (94%)	-0.24	5 (2%)	65	41	31, 55, 117, 188	0
1	B	247/263 (93%)	-0.17	9 (3%)	42	21	37, 60, 120, 176	0
1	C	252/263 (95%)	-0.25	5 (1%)	65	41	34, 56, 120, 164	0
2	D	240/266 (90%)	0.02	12 (5%)	28	12	34, 62, 134, 175	0
2	E	223/266 (83%)	0.00	8 (3%)	42	21	36, 62, 116, 141	0
2	F	230/266 (86%)	-0.05	10 (4%)	35	16	36, 65, 123, 177	0
All	All	1441/1587 (90%)	-0.12	49 (3%)	45	22	31, 60, 122, 188	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	SER	6.2
2	D	311	PRO	5.2
2	D	401	GLN	4.9
2	F	398	ALA	4.2
2	D	532	ALA	3.9
2	D	320	THR	3.8
2	E	287	VAL	3.8
2	E	525	ILE	3.7
2	D	321	GLN	3.5
2	F	529	ALA	3.4
1	B	460	PRO	3.4
2	D	400	ASN	3.2
2	E	520	PRO	3.2
1	A	462	ASP	3.1
1	C	206	GLN	3.1
2	F	515	ASN	3.0
2	E	345	LEU	3.0
2	E	400	ASN	2.9
1	B	462	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	286	ASN	2.8
2	F	335	PRO	2.8
1	B	222	ASP	2.8
1	B	219	LEU	2.7
2	D	319	VAL	2.7
2	E	521	PHE	2.7
1	C	409	SER	2.6
2	F	516	ARG	2.5
1	C	204	MET	2.5
1	C	460	PRO	2.4
1	C	205	VAL	2.4
1	A	460	PRO	2.4
2	D	402	ALA	2.4
2	E	528	VAL	2.4
2	E	516	ARG	2.3
2	D	315	ASP	2.3
2	D	322	THR	2.3
2	F	286	ASN	2.3
1	B	318	SER	2.2
1	B	409	SER	2.2
2	F	513	LEU	2.1
1	A	461	ILE	2.1
1	A	224	SER	2.1
1	B	461	ILE	2.1
2	F	401	GLN	2.1
1	B	305	GLU	2.1
2	F	481	PRO	2.1
1	B	205	VAL	2.1
2	D	287	VAL	2.1
2	F	331	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

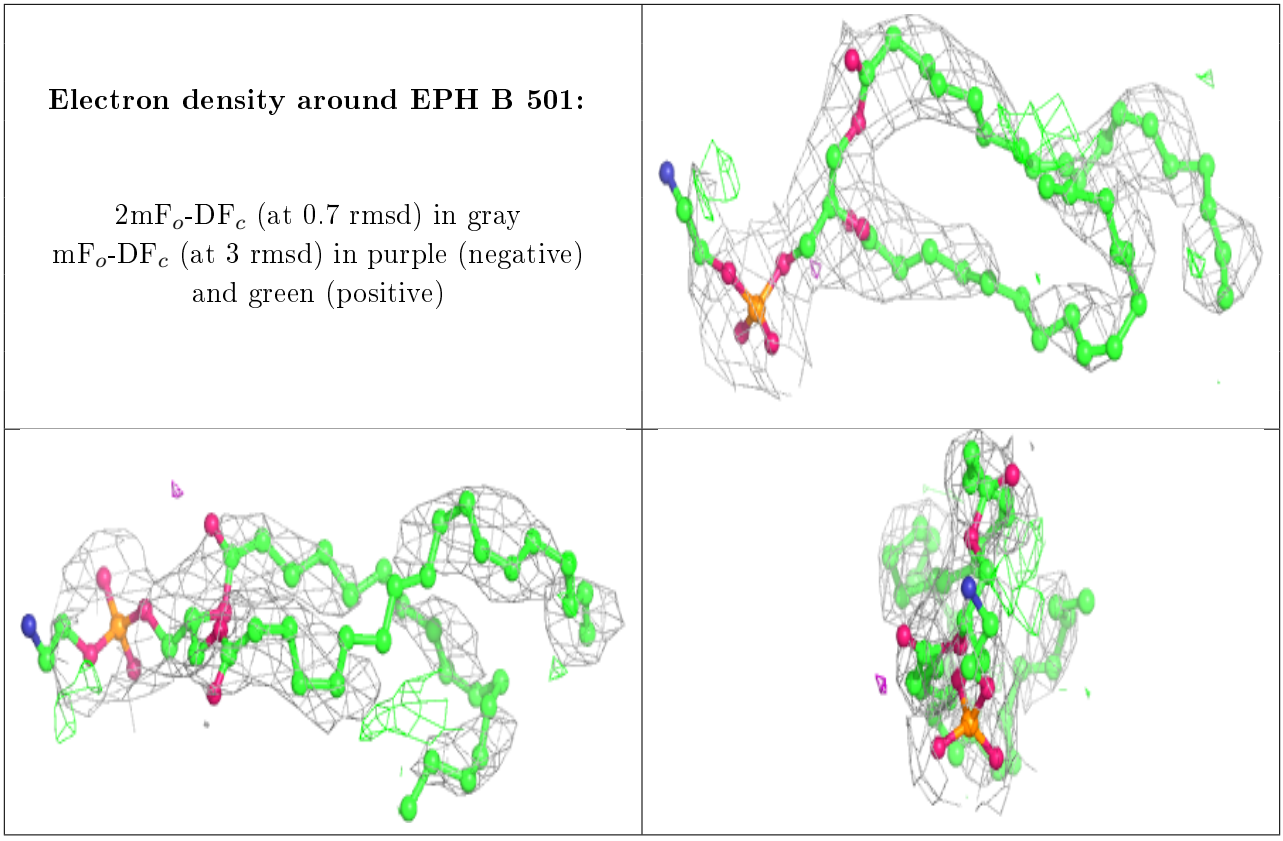
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EPH	B	501	49/49	0.86	0.34	55,78,110,121	0
3	EPH	C	501	49/49	0.87	0.38	38,74,100,109	0
6	PEG	E	602	7/7	0.89	0.20	51,62,66,72	0
5	MG	D	602	1/1	0.90	0.11	46,46,46,46	0
3	EPH	A	501	49/49	0.91	0.30	51,69,93,116	0
6	PEG	F	602	7/7	0.91	0.22	50,52,56,60	7
6	PEG	F	603	7/7	0.91	0.18	63,68,72,82	0
4	U0H	E	601	27/27	0.96	0.26	45,60,73,75	0
4	U0H	D	601	27/27	0.97	0.23	38,46,55,58	0
4	U0H	F	601	27/27	0.97	0.21	51,62,69,71	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.

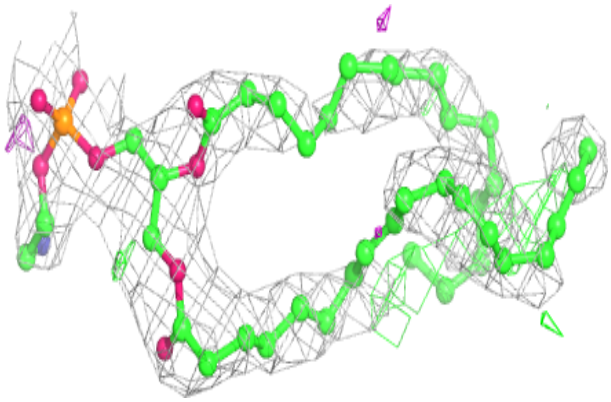
Electron density around EPH B 501:

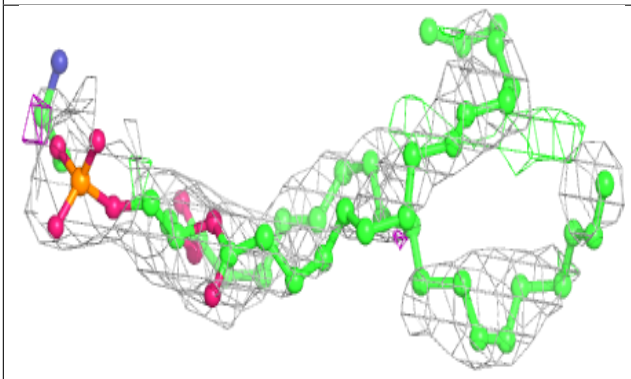
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

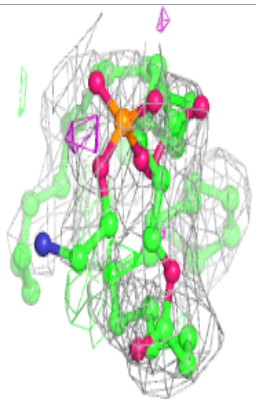


Electron density around EPH C 501:

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

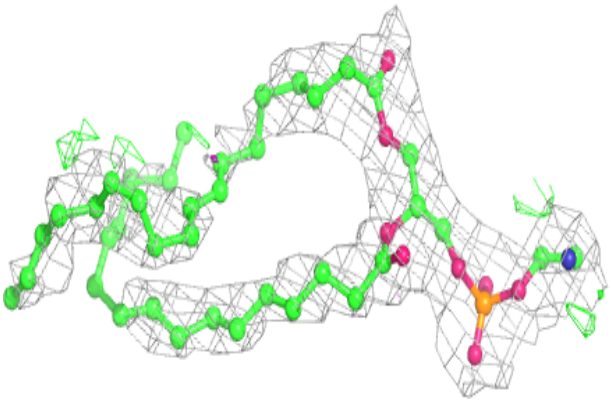


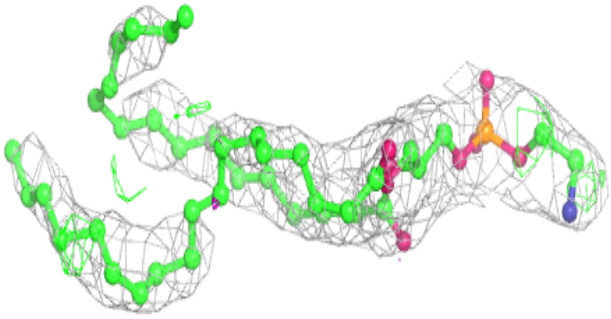


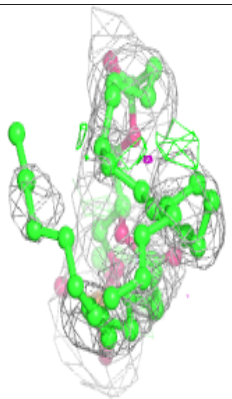


Electron density around EPH A 501:

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

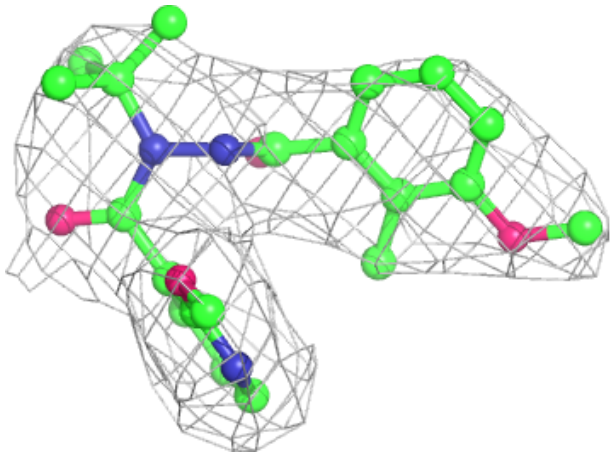


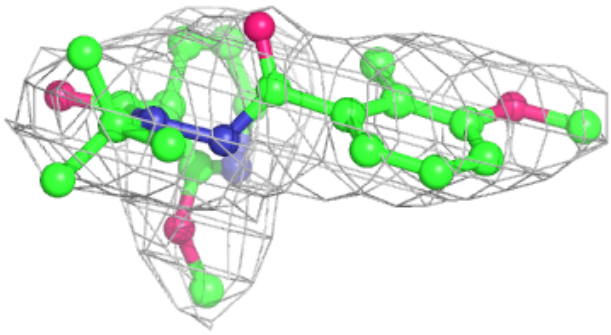


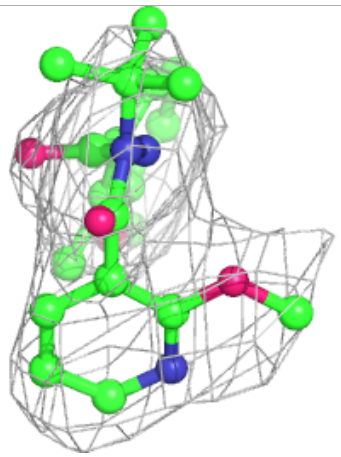


Electron density around U0H E 601:

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

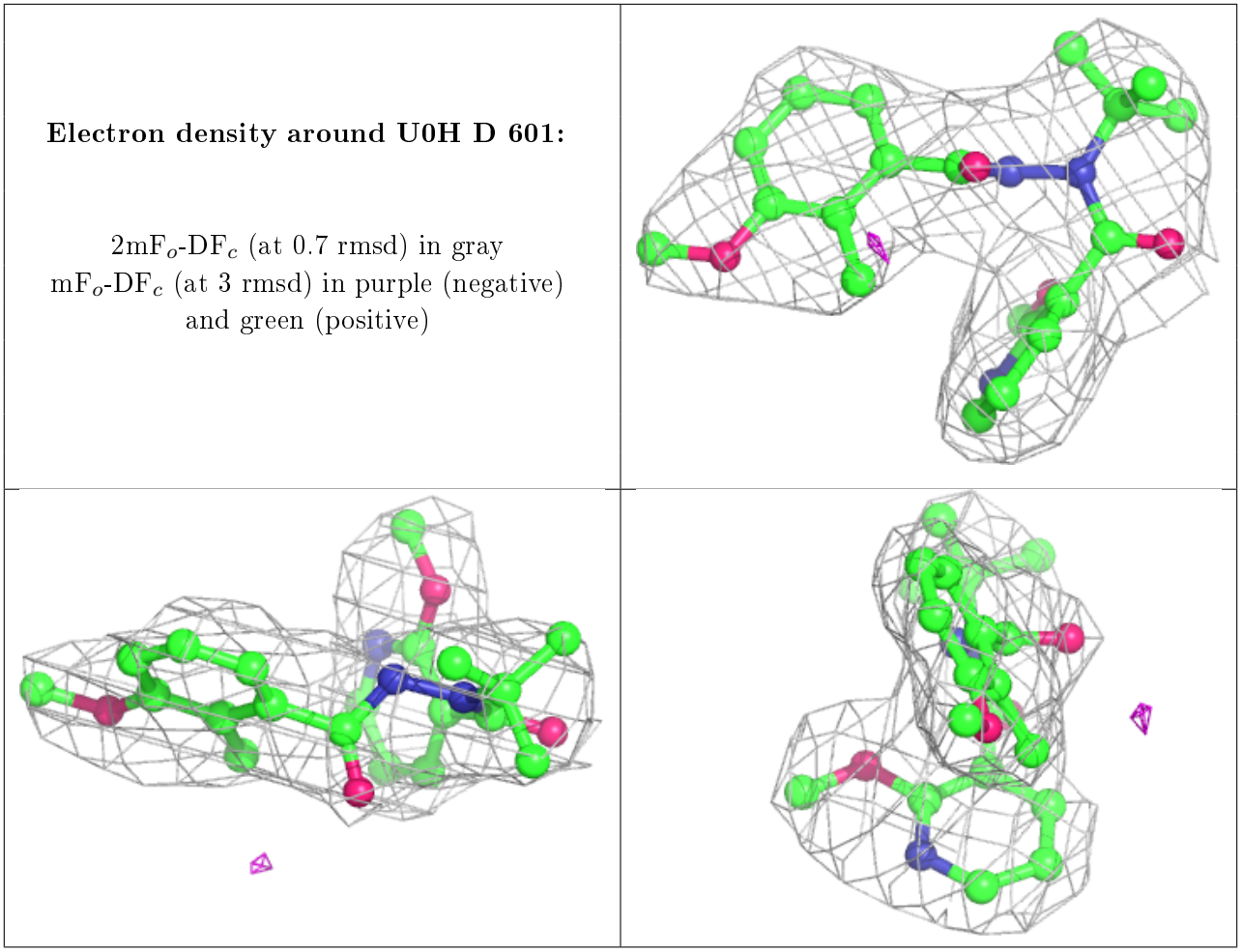






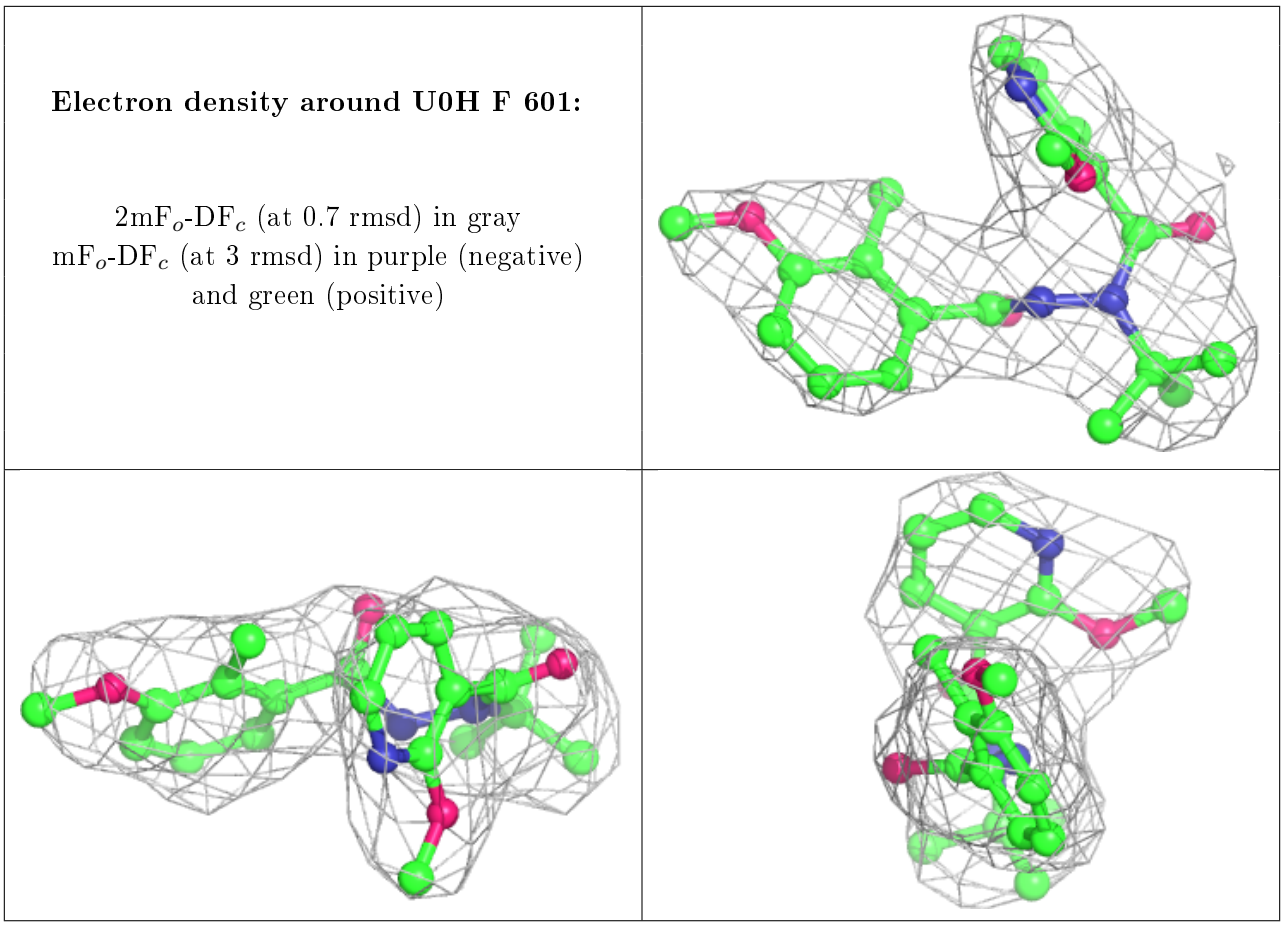
Electron density around U0H D 601:

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



Electron density around U0H 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)



6.5 Other polymers (i)

There are no such residues in this entry.